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Graphs with maximal signless Laplacian spectral radius

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ABSTRACT

By the signless Laplacian of a (simple) graph G we mean the matrix $Q(G) = D(G) + A(G)$, where $A(G), D(G)$ denote respectively the adjacency matrix and the diagonal matrix of vertex degrees of G. It is known that connected graphs G that maximize the signless Laplacian spectral radius $\rho(Q(G))$ over all connected graphs with given numbers of vertices and edges are (degree) maximal. For a maximal graph G with n vertices and r distinct vertex degrees $\delta_r > \delta_{r-1} > \cdots > \delta_1$, it is proved that $\rho(Q(G)) < \rho(Q(H))$ for some maximal graph H with $n+1$ (respectively, n) vertices and the same number of edges as G if either G has precisely two dominating vertices or there exists an integer i, $2 \leqslant i \leqslant \left\lceil \frac{r}{2} \right\rceil$ (respectively, if there exist positive integers i, l with $l + 2 \leqslant i \leqslant \left\lceil \frac{r}{2} \right\rceil$) such that $\delta_i + \delta_{r+1-i} \leqslant n+1$ (respectively, $\delta_i + \delta_{r+1-i} \leqslant \delta_l + \delta_{r-l} + 1$). Graphs that maximize $\rho(Q(G))$ over the class of graphs with m edges and $m-k$ vertices, for $k = 0, 1, 2, 3$, are completely determined.

1. Introduction

For a (simple) graph G, by the *signless Laplacian* of G we mean the matrix $Q(G) = D(G) + A(G)$, where $A(G), D(G)$ denote respectively the adjacency matrix and the diagonal matrix of vertex degrees of G. The matrix $D(G) - A(G)$ is known as the *Laplacian* of G and has been studied extensively in the literature (see, for instance, [7]). The signless Laplacian has appeared rarely in the literature. A very nice reference to this topic is the survey paper [9]. Some people have expressed the view that,

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in comparison to the spectra of other commonly used graph matrices (such as the Laplacian and the adjacency matrix), the signless Laplacian seems to be the most convenient for use in studying graph properties (see [10]). The signless Laplacian is also called the *unoriented Laplacian matrix* by other people and it arose as a special case of the concept of Laplacian matrix of a mixed graph or of a signed graph (see [16,25,26]).

The problem of determining connected graphs (or, graphs) that maximize the spectral radius (or, equivalently, the largest eigenvalue) of the adjacency matrix among all connected graphs (or graphs) with given numbers of vertices and edges is an important classic problem in spectral graph theory. It began with the work of Brualdi and Hoffman [3] in 1985, and was followed by other people [4,21,8,2,19], etc.). The unconnected case of the problem was settled by Rowlinson [21], but the connected case is still unresolved. In [1] four conjectures related to the largest eigenvalue of the adjacency matrix of a graph are posed. The fourth conjecture, which is also given in [22, Problem AWGS.9.], is related to the problem of determining graphs that maximize the largest adjacency eigenvalue among all connected graphs with given number of vertices and edges. These conjectures are considered very hard, and it is noted that resolving the fourth conjecture would be a basis for treating the others.

Research on the signless Laplacian maximizing problem is relatively recent. It began with the work of Fan [13] on the unicyclic case, followed by Fan et al. [14,23] on the bicyclic case and the tricyclic case respectively. The unconnected case and the connected case of the problem are both still open.

An achievement of [23] is to recognize that optimal graphs for the connected case of the signless Laplacian maximizing problem are (degree) maximal graphs – this fact has also been observed independently in [9] – that the concept of neighborhood equivalence classes is relevant, and also to apply the structure theorem of a maximal graph in the study. In [6], the concepts of reduced adjacency matrix and reduced signless Laplacian of a graph are introduced, and counter-examples are provided for a recent conjecture posed by Tam et al. [23] on graphs that maximize the signless Laplacian spectral radius among all (not necessarily connected) graphs with fixed number of vertices and edges. The purpose of this work is to continue the study of graphs that maximize the signless Laplacian spectral radius. We focus mainly on the unconnected case.

Now we describe the contents of this paper briefly. In Section 2, we review some necessary definitions and results that we will need. In Section 3 for a maximal graph G we give conditions which guarantee the existence of a pair of adjacent vertices u, v and a pair of nonadjacent vertices p, q (or, a vertex p of G and a new vertex q) such that the spectral radius of the signless Laplacian of the graph G is less than that of $G - uv + pq$. As a result, we obtain also a set of conditions necessary for a maximal graph to be signless Laplacian maximizing. In Section 4, for a maximal graph G with m edges, we first derive equivalent conditions for $\max\{d(p) + d(q) : pq \in E(G)\} = m + 1 - k$, where k is a given nonnegative integer. When $k = 0, \ldots, 5$, we give the explicit forms of the maximal graphs with m edges for which the said maximum is equal to $m + 1 - k$. Then we determine maximal graphs that maximize the signless Laplacian spectral radius over the class of graphs with m edges and $m - k$ vertices, for $k = 0, \ldots, 3$.

2. Preliminaries

Unless stated otherwise, by a graph we always mean a simple graph, i.e., one without loops nor multiple edges.

Let G be a graph of order n with vertices $v_1, \ldots, v_n$. The *adjacency matrix* of G is the $n \times n$ matrix denoted and given by $A(G) = [a_{ij}]$ where a_{ij} equals 1 or 0 depending on whether vertex v_i and vertex v_j are adjacent or not. The *signless Laplacian* of G is the $n \times n$ matrix given by $Q(G) = D(G) + A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees of G. (In [14,23], the signless Laplacian of G is called the *unoriented Laplacian matrix* of G and is denoted by $K(G)$.) The signless Laplacian of G can also be defined, equivalently, as $M(G)M(G)^T$, where $M(G) = (m_{ij})$ is the (vertex–edge, unoriented) *incidence matrix* of G.

We denote by $\rho(B)$ the spectral radius of a (square) matrix B. For a graph G, since $Q(G)$ is a (entrywise) nonnegative, positive semidefinite matrix, it is clear that $\rho(Q(G))$ is equal to the largest eigenvalue of $Q(G)$.

When it is clear from the context, we often omit the dependence on G and denote $A(G)$, $D(G)$, $Q(G)$ simply by A, D and Q respectively.

We refer to the eigenvalues, the spectral radius, the spectrum and the characteristic polynomial of $Q(G)$ as the signless Laplacian eigenvalues, signless Laplacian spectral radius, the signless Laplacian spectrum and the signless Laplacian characteristic polynomial of G. The terms Q-eigenvalues, largest Q-eigenvalue, Q-spectrum and Q-polynomial have also been used in the literature for these objects (see, for instance, [9]).

For a vertex u of G we denote by $N_G(u)$ (or simply $N(u)$ when there is no danger of confusion) the set of neighbors of u in G, i.e. $N_G(u) := \{v \in V(G) : uv \in E(G)\}$.

We define relations $\geqslant^G$ and $\sim^G$ on $V(G)$ by

$$u \overset{G}{\geqslant} v \text{ if and only if } N(u)\backslash\{v\} \supseteq N(v)\backslash\{u\}$$

and

$$u \sim^G v \text{ if and only if } N(u)\backslash\{v\} = N(v)\backslash\{u\}.$$

It is straightforward to verify (see, for instance, [23]) that the relation $\geqslant^G$ is a pre-order, i.e. $\geqslant^G$ is reflexive and transitive, and $\sim^G$ is an equivalence relation. In the literature, the pre-order $\geqslant^G$ on $V(G)$ is called the *vicinal pre-order* of G (see [18]) and the relation $\sim^G$ is called the *neighborhood equivalence relation* on G (see [5]). The equivalence classes for $\sim^G$ will be referred to as the *neighborhood equivalence classes* of G.

We denote the cardinality of a set S by $|S|$. For every positive integer n, we use $\langle n\rangle$ to stand for the set $\{1, \ldots, n\}$.

Now we define the concepts of reduced adjacency matrix and reduced signless Laplacian as introduced in [6].

Let G be a graph with neighborhood equivalence classes $V_1, \ldots, V_r$. From the definition of $\sim^G$ it is readily seen that each V_i is either a clique or a stable set. Moreover, for any $i, j \in \langle r\rangle$, $i \neq j$, either each vertex of V_i is adjacent to every vertex of V_j or there is no edge between vertices of V_i and vertices of V_j. For $i, j \in \langle r\rangle$, let γ_{ij} equal 1 if there is at least one edge between a vertex of V_i and a vertex of V_j and equal 0, otherwise. By the *reduced adjacency matrix* of G we mean the $r \times r$ matrix $B(G) = [b_{ij}]$ given by: b_{ii} equals $\gamma_{ii}(n_i - 1)$ and b_{ij} equals $\gamma_{ij}n_j$ for $i \neq j$. By definition, vertices in the same V_i share a common degree, which we denote by δ_i. Let $\Delta(G)$ denote the $r \times r$ diagonal matrix $\mathrm{diag}(\delta_1, \ldots, \delta_r)$. We call the $r \times r$ matrix $\Delta(G) + B(G)$ the *reduced signless Laplacian* of G and abbreviate it as $(\Delta + B)(G)$. When there is no danger of confusion, we write B, Δ and $\Delta + B$ for $B(G)$, $\Delta(G)$ and $(\Delta + B)(G)$ respectively. The terms reduced signless Laplacian eigenvalues, reduced signless Laplacian spectrum and reduced signless Laplacian characteristic polynomial are used with the obvious meanings.

The characteristic polynomial of the signless Laplacian $Q(G)$ and that of the reduced signless Laplacian $(\Delta + B)(G)$ of G will be denoted by $Q_G(x)$ and $q_G(x)$ respectively.

It is known that regular graphs can be recognized, and their degree and the number of components calculated, from $Q_G(x)$ (see [10] or [9, Proposition 3.1]). A formula for $q_G(x)$ when G is a (degree) maximal graph can be found in [24, in this issue]. (The definition of a maximal graph will be given shortly.)

In [6], a theorem on the spectrum of a special kind of block-stochastic matrices is obtained and applied to various graph matrices. In particular, for the signless Laplacian of a graph we have the following:

Theorem 2.1. *Let G be a graph with neighborhood equivalence classes $V_1, \ldots, V_r$. For each $i = 1, \ldots, r$, denote by n_i the cardinality of V_i and by δ_i the common degree of the vertices in V_i. Let $I_1 = \{i \in \langle r\rangle : n_i > 1$ and V_i is a stable set$\}$, and $I_2 = \{i \in \langle r\rangle : n_i > 1$ and V_i is a clique$\}$. Then*

$$\sigma(Q(G)) = \sigma((\Delta + B)(G)) \cup \{\delta_i^{n_i-1} : i \in I_1\} \cup \{(\delta_i - 1)^{n_i-1} : i \in I_2\},$$

where the exponents indicate multiplicities, and

$$\rho(Q(G)) = \rho((\Delta + B)(G));$$

hence we have

$$Q_G(x) = q_G(x) \prod_{i \in I_1} (x - \delta_i)^{n_i - 1} \prod_{i \in I_2} (x - \delta_i + 1)^{n_i - 1}. \tag{2.1}$$

Note that the roots of the polynomial $q_G(x)$ are all nonnegative, being part of the eigenvalues of the positive semidefinite matrix $Q(G)$. In fact, they are all positive, unless G has a bipartite component, because it is known that the least eigenvalue of the signless Laplacian of a connected graph is equal to 0 if and only if the graph is bipartite (see [9, Proposition 2, 1]).

We are particularly interested in maximal graphs and threshold graphs, as they are respectively candidates for graphs that maximize the signless Laplacian spectral radius over connected graphs or graphs with given numbers of vertices and edges.

A graph $G = (V, E)$ is called a *threshold graph* if there exist nonnegative real numbers $w_v, v \in V$ (the vertex-weights) and a real number t (the threshold) such that for any subset U of V, U is a stable set if and only if $\sum_{v \in U} w_v \leqslant t$.

If $\alpha = (a_1, \ldots, a_r)$ and $\beta = (b_1, \ldots, b_s)$ are two (finite) sequences of real numbers, then we say α *majorizes* β if $\sum_{i=1}^{k} a_i^{\downarrow} \geqslant \sum_{i=1}^{k} b_i^{\downarrow}$ for $k = 1, \ldots, \min\{r, s\}$ and $\sum_{i=1}^{r} a_i = \sum_{i=1}^{s} b_i$, where $a_1^{\downarrow}, \ldots, a_r^{\downarrow}$ is a rearrangement of $a_1, \ldots, a_r$ in nonincreasing order.

Following Merris [17], we call a graph (degree) *maximal* if it is connected and its degree sequence is not majorized by that of other connected graph.

It can be shown that a connected graph is maximal if and only if it is threshold; a threshold graph that is not connected must be the (disjoint) union of a maximal graph and a null (i.e. edgeless) graph. There are many known equivalent conditions for a graph G to be threshold (see [15] or [18]). One equivalent condition is that the vicinal pre-order of G is total.

If G is a maximal graph, then the total pre-order $\geqslant^G$ on $V(G)$ induces in a natural way a total partial order on the quotient set $V(G)/\sim^G$. Let $V_1, \ldots, V_r$ denote the neighborhood equivalence classes of G, arranged in strict ascending order with respect to the total partial order. It can be shown that, in this case, for any $i, j \in \langle r \rangle$, there are edge(s) between V_i and V_j if and only if $i + j \geqslant r + 1$. So the structure of a maximal graph G – that is, how the edges link the various neighborhood equivalence classes, and whether an equivalence class is a clique or a stable set – is completely determined (up to isomorphism) once the cardinalities of the neighborhood equivalence classes are specified. In [23] the symbol $C(n_1, \ldots, n_r)$ is introduced to denote a maximal graph with neighborhood equivalence classes $V_1, \ldots, V_r$, arranged in strict ascending order with respect to the total partial order induced by the vicinal pre-order of the graph, such that the cardinality of V_i is n_i for $i = 1, \ldots, r$. Here $n_1, \ldots, n_r$ can be any positive integers except that we need to require $n_{\lceil \frac{r}{2} \rceil} \geqslant 2$. (For a fuller discussion, we refer the reader to [23, Sections 3 and 4].)

Hereafter, for the maximal graph $C(n_1, \ldots, n_r)$, we will use $V_1, \ldots, V_r$ to denote its neighborhood equivalence classes, with the same meaning as mentioned above. Note that for each $i \in \langle r \rangle$, V_i is a clique if and only if $i \geqslant \left\lceil \frac{r+1}{2} \right\rceil$. Moreover, V_r is composed of the *dominating vertices*, i.e., vertices that are adjacent to every other vertex of the graph. Unless specified otherwise, we also use δ_i to denote the common degree of the vertices in V_i for $i = 1, \ldots, r$. Making use of the structure of a maximal graph, one can express the δ_i's in terms of the n_i's in the following way:

$$\delta_i = \begin{cases} \sum\limits_{j=r+1-i}^{r} n_j & \text{for } 1 \leqslant i \leqslant \left\lfloor \frac{r}{2} \right\rfloor \\ \sum\limits_{j=r+1-i}^{r} n_j - 1 & \text{for } \left\lfloor \frac{r}{2} \right\rfloor < i \leqslant r \end{cases}. \tag{2.2}$$

Conversely, the n_i's can also be expressed in terms of the δ_i's as follows:

$$n_i = \delta_{r+1-i} - \delta_{r-i} \quad \text{for } i = 1, \ldots, r, i \neq \left\lceil \frac{r}{2} \right\rceil \quad \text{and} \quad n_{\lceil \frac{r}{2} \rceil} = \delta_{\lceil \frac{r+1}{2} \rceil} - \delta_{\lfloor \frac{r}{2} \rfloor} + 1, \tag{2.3}$$

where δ_0 is taken to be 0.

By relations (2.2) and (2.3) and the fact that $n_i \geqslant 1$ for each i and $n_{\lceil \frac{r}{2} \rceil} \geqslant 2$, one readily shows that

$$\delta_i \geqslant i \quad \text{for } i = 1, \ldots, r-1. \tag{2.4}$$

(Of course, $\delta_r = d_{\max}(G) = n-1$, where $d_{\max}(G)$ denotes the largest degree of a vertex in G.)

The maximal graph $C(n_1, \ldots, n_r)$ clearly has $n_1 + \cdots + n_r$ vertices. Since the sum of degrees of a graph is equal to twice of its number of edges, $C(n_1, \ldots, n_r)$ has altogether $\frac{1}{2}\sum_{i=1}^{r} n_i\delta_i$ edges. Often it is more convenient to express the number of edges of $C(n_1, \ldots, n_r)$ in another way as follows. We count, for each $j = \left\lceil \frac{r+1}{2} \right\rceil$, the number of edges between V_j and V_i for $i \leqslant j$ and then take the sum. This gives

$$|E(C(n_1, \ldots, n_r))| = \sum_{j=\lceil \frac{r+1}{2} \rceil}^{r} \left[n_j \sum_{i=r+1-j}^{j-1} n_i + \binom{n_j}{2} \right].$$

For vertex-disjoint graphs G, H, we use $G \cup H$ to denote their (disjoint) *union*. For such pair of graphs, their join, $G \vee H$, is the graph obtained from $G \cup H$ by joining each vertex of G to every vertex of H.

If G is a graph on n vertices, we denote by G^c the complement of G (in the complete graph K_n). So a null graph of order n can be written as K_n^c. For convenience, we use K_0 or K_0^c to stand for the empty graph (i.e., one without vertices or edges) and adopt the convention $G \cup K_0 = G$ and $G \vee K_0 = G$.

The following known result is fundamental to this topic (see, [9, Theorems 6.3 and 6.3′] or [23, Theorem 5.4]; for an extension of the result, see [6]):

Lemma 2.2. *Every graph that maximizes the signless Laplacian spectral radius over all graphs* (*respectively, connected graphs*) *with given numbers of vertices and edges is a threshold graph* (*respectively, maximal graph*).

3. Effects of edge replacement on the signless Laplacian spectral radius

The question of which single edges can be added to or deleted from a given threshold graph to obtain another threshold graph has occurred to Peled and Srinivasan [20] in their study of the polytope of degree sequences. They give the answer in terms of the concept of split partition. Fan [11,12] in his study of spectral integral variations of the Laplacian matrix has also treated the question of when the addition of an edge to a maximal graph does not affect the maximality of the graph, and gave the answer in terms of the degree sequence of the underlying graph. In [23, Section 7] the same question has been reconsidered in the light of the structure theorem for a maximal graph.

In this section we will answer the following question: If G is a maximal graph, u, v is a pair of adjacent vertices, and p, q is a pair of nonadjacent vertices of G (or p is a vertex of G and q is a new vertex), when is the graph $G - uv + pq$ maximal? And when there exist such pairs u, v and p, q such that $G - uv + pq$ is a maximal graph that satisfies $\rho(Q(G - uv + pq)) > \rho(Q(G))$?

We find it convenient to introduce some new terms.

Let G be a threshold graph with neighborhood equivalence classes $V_0, V_1, \ldots, V_r$, where V_0 (which is possibly empty) denotes the class consisting of the isolated vertices of G and V_i denotes the class consisting of vertices with common degree δ_i, $\delta_r > \cdots > \delta_1$ being the distinct positive vertex-degrees of G. A pair of adjacent vertices u, v of G is said to form *a complementary pair of adjacent vertices* if there exists i, $1 \leqslant i \leqslant r$ such that $u \in V_i$ and $v \in V_{r+1-i}$. A pair of nonadjacent (distinct) vertices u, v is said to form *a complementary pair of nonadjacent vertices* if there exists i, $0 \leqslant i \leqslant r$ such that $u \in V_i$ and $v \in V_{r-i}$.

As an illustration of these newly introduced concepts, consider a maximal graph G and a null graph K_p^c whose vertex set is disjoint from that of G. Take a dominating vertex x of G and any vertex y of K_p^c. Then x, y form a complementary pair of nonadjacent vertices of the threshold graph $G \cup K_p^c$. If K_q is a complete graph whose vertex set is disjoint from that of the latter threshold graph, then x, y still form a complementary pair of nonadjacent vertices of the maximal graph $(G \cup K_p^c) \vee K_q$.

By [23, Theorems 7.2 and 7.3] we have the following:

Remark 3.1. For a pair of distinct nonadjacent vertices u, v of a threshold (respectively, maximal) graph G, $G + uv$ is threshold (respectively, maximal) if and only if u, v form a complementary pair of nonadjacent vertices.

Lemma 3.2. *Let G be a threshold graph. If u, v form a complementary pair of nonadjacent vertices of G, then u, v also form a complementary pair of nonadjacent vertices of the maximal graph $(G \cup K_p^c) \vee K_q$, where p, q are any positive integers.*

Proof. First, consider the case when p, q are both positive integer. Let $V_0, \ldots, V_r$ denote the neighborhood equivalence classes of the threshold graph G (with the usual meaning). Then $(G \cup K_p^c) \vee K_q$ is a maximal graph with $r + 2$ neighborhood equivalence classes $V_1', \ldots, V_{r+2}'$ given by: $V_1' = V_0 \cup V(K_p)$, $V_i' = V_{i-1}$ for $i = 2, \ldots, r + 1$ and $V_{r+2}' = V(K_p)$. Let u, v be a complementary pair of nonadjacent vertices of G. We have $u \in V_i$ and $y \in V_j$ for some i, j, $0 \leqslant i, j \leqslant r$. But $V_i \subseteq V_{i+1}'$, $V_j \subseteq V_{j+1}'$ and $(i + 1) + (j + 1) = r + 2$, so x, y also form a complementary pair of nonadjacent vertices of $(G \cup K_p^c) \vee K_q$. $\square$

In fact, Lemma 3.2 still holds when p or q (or both) equals 0. (Recall that by convention K_0 and K_0^c both stand for the null graph.)

Lemma 3.3. *Let G be a maximal graph and let $V_1, \ldots, V_r (r \geqslant 2)$ be the neighborhood equivalence classes of G. Let $u \in V_r$ and $v \in V_1$. Then:*

(i) *$G - uv$ is a maximal graph if $|V_r| \geqslant 2$ and is a threshold graph if $|V_r| = 1$.*
(ii) *If $|V_r| \geqslant 2$, then the dominating vertices of V other than u remain dominating vertices in $G - uv$.*
(iii) *If x, y form a complementary pair of nonadjacent vertices of G and if neither of them equals v, then x, y also form a complementary pair of nonadjacent vertices of $G - uv$.*

Proof. Let G be the maximal graph $C(n_1, \ldots, n_r)$. As can be readily checked, we have

$$G - uv = \begin{cases} C(1, n_1 - 1, n_2, \ldots, n_{r-1}, 1, n_r - 1) & \text{if } n_r \geqslant 2 \text{ and } n_1 \geqslant 2, \\ C(n_1, n_2, \ldots, n_{r-1} + 1, n_r - 1) & \text{if } n_r \geqslant 2 \text{ and } n_1 = 1, \\ C(n_1 - 1, n_2, \ldots, n_{r-1}, n_r) \cup K_1 & \text{if } n_r = 1 \text{ and } n_1 \geqslant 2, \\ C(n_2, n_3, \ldots, n_{r-2}, n_{r-1} + 1) \cup K_1 & \text{if } n_r = 1 \text{ and } n_1 = 1. \end{cases}$$

So it is clear that (i) holds. To establish (ii) and (iii), we have to examine closely the neighborhood equivalence classes of $G - uv$. In below we treat the most general case when $n_r \geqslant 2$ and $n_1 \geqslant 2$, the argument for the other cases being similar. In this case, the maximal graph $G - uv$ has $r + 2$ neighborhood equivalence classes, say, $V_1', V_2', \ldots, V_{r+2}'$, arranged in strict ascending order with respect to the total partial order induced by the vicinal pre-order of G. Then we have

$$V_{r+2}' = V_r \setminus \{u\}, \quad V_{r+1}' = \{u\}, \quad V_j' = V_{j-1} \text{ for } j = 3, \ldots, r, \quad V_2' = V_1 \setminus \{v\} \text{ and } V_1' = \{v\}.$$

Since $V_{r+2}' = V_r \setminus \{u\}$, (ii) clearly follows. Let x, y be a complementary pair of nonadjacent vertices of G, both different from v; say, $x \in V_{r-i}, y \in V_i, r - i \geqslant i (\geqslant 1)$. Clearly, $x \notin V_r$, so $r - 1 \geqslant r - i$ and we have $x \in V_{r-i+1}'$. Similarly, we also have $y \in V_{i+1}'$. But $(r - i + 1) + (i + 1) = r + 2$, so x, y form a complementary pair of nonadjacent vertices of $G - uv$. $\square$

It is straightforward to show the following:

Remark 3.4. Let G, H be vertex-disjoint graphs.

(i) For any pair of adjacent vertices u, v of G, we have

$$(G \cup H) - uv = (G - uv) \cup H \quad \text{and} \quad (G \vee H) - uv = (G - uv) \vee H.$$

(ii) For any pair of nonadjacent vertices p, q of G, we have

$$(G \cup H) + pq = (G + pq) \cup H \quad \text{and} \quad (G \vee H) + pq = (G + pq) \vee H.$$

Let G be a threshold graph and let u, v be a complementary pair of adjacent vertices of G (so that $G - uv$ is still a threshold graph). It is straightforward to verify that if x, y form a complementary pair of nonadjacent vertices of G and x, y are both different from u, v, then x, y also form a complementary pair of nonadjacent vertices of $G - uv$.

By an *alternating 4-cycle* of a graph G we mean a configuration consisting of distinct vertices a, b, c, d of G such that $ab, cd \in E(G)$ and $ac, bd \notin E(G)$. One characterization of a threshold graph, which we are going to make use of, is that the graph does not have an alternating 4-cycle.

Lemma 3.5. *Let G be a maximal graph with r neighborhood equivalence classes. Let uv be an edge of G. Then $G - uv$ is a maximal graph if and only if one of the following holds:*

(a) *$r = 1$ and $G \neq K_1, K_2$.*
(b) *$r \geqslant 2$, one of the vertices u, v is a dominating vertex and the other is a vertex of least degree, and G has two or more dominating vertices.*
(c) *$r > 2$, none of the vertices u, v is a dominating vertex and u, v form a complementary pair of adjacent vertices.*

When the equivalent conditions are satisfied, every complementary pair of nonadjacent vertices of G, which is composed of vertices different from u, v, forms a complementary pair of nonadjacent vertices of $G - uv$.

Proof. Let $V_1, \ldots, V_r$ denote the neighborhood equivalence classes of G with the usual meaning.

"Only if" part: Suppose that $G - uv$ is a maximal graph. If $r = 1$, it is clear that $G \neq K_1, K_2$. Hereafter, assume that $r \geqslant 2$. If one of the vertices u, v is a dominating vertex and the other is a vertex of least degree, then by Lemma 3.3 G has two or more dominating vertices. So suppose that u, v do not form a complementary pair of adjacent vertices. Then there exist $i, j \in \langle r \rangle$ with $i + j > r + 1$ such that $u \in V_i$ and $v \in V_j$. Take any vertex $x \in V_{r+1-i}$ and $y \in V_{i-1}$. Since $(i - 1) + j \geqslant r + 1$, vy is an edge of G and hence also an edge of $G - uv$. Clearly, $ux \in E(G - uv)$ and $uv \notin E(G - uv)$. On the other hand, we also have $yx \notin E(G - uv)$ as $(i - 1) + (r + 1 - i) = r < r + 1$. So the graph $G - uv$ contains an alternating 4-cycle consisting of the vertices u, x, v, y and hence is not a maximal graph.

"If" part and the last part: If $r = 1$ and $G \neq K_1, K_2$ then $G = K_n$ for some $n \geqslant 3$, in which case $G - uv$ is the maximal graph $C(2, n - 2)$. (In this case G does not have a pair of nonadjacent vertices. So we need not consider the last part of the lemma.) If condition (b) is satisfied, then by Lemma 3.3 $G - uv$ is a maximal graph and the last part of this lemma also follows.

Now we treat the remaining condition (c). Suppose that we have $u \in V_i, v \in V_j$ and $i \geqslant j$. Clearly $j \geqslant 2$. Let $G = C(n_1, \ldots, n_r)$. Consider the chain of maximal graphs $C(n_{j-t}, \ldots, n_{i+t})$, $t = 0, \ldots, j - 1$, which begins with $C(n_j, \ldots, n_i)$ and ends with G. Note that for $t = 1, \ldots, j - 1$, we have

$$C(n_{j-t}, \ldots, n_{i+t}) = \left(C(n_{j-t+1}, \ldots, n_{i+t-1}) \cup K^c_{n_{j-t}}\right) \vee K_{n_{i+t}}.$$

By Remark 3.4, for t in such range we also have

$$C(n_{j-t}, \ldots, n_{i+t}) - uv = \left((C(n_{j-t+1}, \ldots, n_{i+t-1}) - uv) \cup K^c_{n_{j-t}}\right) \vee K_{n_{i+t}}.$$

Since u is a dominating vertex and v is a vertex with least degree in the maximal graph $C(n_j, \ldots, n_i)$, by Lemma 3.3 $C(n_j, \ldots, n_i) - uv$ is a threshold graph. (If $i = j = \frac{r+1}{2}$ with odd r, then $C(n_j, n_{j+1}, \ldots, n_i) - uv$ becomes $K_{n_{\frac{r+1}{2}}} - uv$, which is still a threshold graph.) It is clear that if we form a new graph from a threshold graph by first taking union with a null graph and then taking join with a complete graph then the resulting graph is a maximal graph. So $C(n_{j-1}, \ldots, n_{i+1}) - uv$ is a maximal graph. Proceeding in this way, we can conclude that $G - uv$ is a maximal graph.

It remains to show that every complementary pair of nonadjacent vertices of G, which is composed of vertices different from u, v, is also a complementary pair of nonadjacent vertices of $G - uv$. Let x, y be a complementary pair of nonadjacent vertices of G such that x, y are both different from u, v; say, $x \in V_p, y \in V_{r-p}$ with $p \geqslant r - p$. First, consider the case when $p < i$. Then x, y are both vertices of $C(n_j, \ldots, n_i)$ and form a complementary pair of nonadjacent vertices of $C(n_j, \ldots, n_i)$. By Lemma 3.3 x, y also form a complementary pair of nonadjacent vertices of $C(n_j, \ldots, n_i) - uv$. Since $C(n_{j-1}, \ldots, n_{i+1}) - uv = ((C(n_j, \ldots, n_i) - uv) \cup K^c_{n_{j-1}}) \vee K_{n_{i+1}}$, by Lemma 3.2 x, y also form a complementary pair of nonadjacent vertices of $C(n_{j-1}, \ldots, n_{i+1}) - uv$. Proceeding in this way, we can conclude that x, y form a complementary pair of nonadjacent vertices of $G - uv$.

Now suppose $p = i$. Since $x \neq u$, we have $|V_i| \geqslant 2$, and by the last part of Lemma 3.3, x is a dominating vertex of $C(n_j, \ldots, n_i) - uv$. Since y belongs to V_{j-1} (as $r - p = j - 1$) and $C(n_{j-1}, \ldots, n_{i+1}) - uv$ can be formed from $C(n_j, \ldots, n_i) - uv$ by first taking union with $K^c_{n_{j-1}}$ and then taking join with K_{i+1}, it is clear that x, y form a complementary pair of nonadjacent vertices of $C(n_{j-1}, \ldots, n_{i+1}) - uv$. Applying Lemma 3.2 repeatedly, we can conclude that x, y also form a complementary pair of nonadjacent vertices of $G - uv$.

It remains to consider the case when $p > i$. As before, $C(n_j, \ldots, n_i) - uv$ is a threshold graph, but $C(n_{j-t}, \ldots, n_{i+t}) - uv$ is a maximal graph for $t = 1, \ldots, r - i$. In particular, if we take $t = p - i$, then since $j - t = (r + 1 - i) - (p - i) = r + 1 - p$, we find that $C(n_{r+1-p}, \ldots, n_p) - uv$ is a maximal graph. Since $x \in V_p$, x is a dominating vertex of the latter maximal graph. As $C(n_{r-p}, \ldots, n_{p+1}) - uv = ((C(n_{r+1-p}, \ldots, n_p) - uv) \cup K^c_{n_{r-p}}) \vee K_{n_{p+1}}$ and $y \in V_{r-p}$, it follows that x, y form a complementary pair of nonadjacent vertices of $C(n_{r-p}, \ldots, n_{p+1}) - uv$. Applying Lemma 3.2 repeatedly, we can conclude that x, y also form a complementary pair of nonadjacent vertices of $G - uv$. The proof is complete. $\square$

Theorem 3.6. *Let G be a maximal graph with n vertices and r neighborhood equivalence classes $V_1, \ldots, V_r$, $r \geqslant 2$. Let $\delta_r > \delta_{r-1} > \cdots > \delta_1$ be the distinct vertex degrees of G. Let i be an index less than or equal to $\left\lceil \frac{r}{2} \right\rceil$. Suppose that $i \geqslant 2$ and $\delta_i + \delta_{r+1-i} \leqslant n + 1$ or $i = 1$ and G has precisely two dominating vertices. Let $u \in V_{r+1-i}$, $v \in V_i$, $p \in V_r$ and with $p \neq u$ in case $i = 1$, and let q be a new vertex. Let H be the graph obtained from G by deleting the edge uv and adding the edge pq, i.e., $H = G - uv + pq$. Then H is a maximal graph and $\rho(Q(G)) < \rho(Q(H))$.*

Proof. First, in view of Lemma 3.5 $\left(\text{using condition (b) when } i = 1 \text{ and condition (c) when } 2 \leqslant i \leqslant \left\lceil \frac{r}{2} \right\rceil\right)$, $G - uv$ is a maximal graph. Now p, q form a complementary pair of nonadjacent vertices of the threshold graph obtained from G by adding the isolated vertex q and they still form a complementary pair of nonadjacent vertices of the threshold graph obtained from $G - uv$ by adding the isolated vertex q. In view of Remark 3.1 $G - uv + pq$, i.e., H, is a connected threshold and hence a maximal graph.

Let x be the Perron vector of $Q(G)$ and let $y = M(G)^T x$. It is known that y is the Perron vector of $A(L_G)$ (see, for instance, [9, the beginning of Section 4]). Index the components of x by the vertices of G, i.e., let x_u denote the component x_i of x if u stands for the vertex v_i of G. Also, index the components of y by the edges of G. Then we have $y_e = x_u + x_v$ if e is the edge uv.

Our strategy is to show that $y^T A(L_H) y - y^T A(L_G) y > 0$. Once this is proved, the desired inequality $\rho(Q(G)) < \rho(Q(H))$ will follow, as $\rho(Q(G)) = \rho(A(L_G)) + 2$ and we have

$$\rho(A(L_H)) \geqslant z^T A(L_H) z > z^T A(L_G) z = \rho(A(L_G)),$$

where we use z to denote the unit Perron vector $\frac{y}{\|y\|}$ of G. (But if we obtain only $y^T A(L_H) y - y^T A(L_G) y = 0$, then we have to play with the eigenvector equations of $A(L_G)$ and $A(L_H)$.)

Using the definition of the adjacency matrix, we have $y^T A(L_G) y = 2 \sum y_e y_f$, where the sum is taken over all pairs of incident edges e, f of G. A similar expression also holds for $y^T A(L_H) y$. In evaluating $y^T A(L_H) y$ we index the components of y by the vertices of L_H. The components of y corresponding to vertices of L_H other than pq take the same values as before, but the component y_{uv} is now associated with the vertex pq (instead of uv). Since H is obtained from G by replacing the edge uv by the edge pq, we have

$$y^TA(L_H)y - y^TA(L_G)y = 2y_{uv}\left[\sum_{e\in N_{L_H}(pq)} y_e - \sum_{e\in N_{L_G}(uv)} y_e\right]. \tag{3.1}$$

We divide our discussion into three cases according to $i = 1$ (with $|V_r| = 2$), $1 < i < \frac{r+1}{2}$, or $i = \frac{r+1}{2}$ (with r odd).

For $j = 1,\ldots,r$, denote $|V_j|$ by n_j. It is known that if u, v belong to the same neighborhood equivalence class of G then the corresponding components x_u, x_v of the Perron vector x are the same (see [23, Lemma 3.2(ii)]). Let ξ_i be the common value of x_u for $u \in V_i$. Denote the vector $(\xi_1,\ldots,\xi_r)^T$ by ξ and $\rho(Q(G))$ by ρ. Then the eigenvector equation $Q(G)x = \rho x$ can be rewritten as $(\Delta + B)\xi = \rho\xi$, i.e., ξ is the Perron vector of $\Delta + B$.

Case 1: $i = 1$ (with $|V_r| = 2$). Since q is a pendant vertex and p is a dominating vertex of H, we have

$$\sum_{e\in N_{L_H}(pq)} y_e = \sum_{w\in V(G)\setminus\{p\}} y_{pw} = \sum_{w\in V(G)\setminus\{p,u,v\}} (x_p + x_w).$$

On the other hand, we also have

$$\sum_{e\in N_{L_G}(uv)} y_e = \sum_{w\in V(G)\setminus\{u,v\}} (x_u + x_w) + (x_p + x_v)$$

noting that pv is the only edge of G that is incident with uv at v. As $x_p = x_u$, it follows that the right side of (3.1) is equal to 0. Hence $z^TA(L_H)z - z^TA(L_G)z = 0$ where $z = \frac{y}{\|y\|}$ is the unit Perron vector of $A(L_G)$. Then we have $\rho(A(L_G)) = z^TA(L_G)z = z^TA(L_H)z \leqslant \rho(A(L_H))$. If the latter inequality is an equality, then z is also the unit Perron vector of $A(L_H)$. So we have $(A(L_G) - A(L_H))y = 0$. To carry out calculations, we denote the edges of G as $e_1,\ldots,e_m$ with $e_m = uv$, and denote the edges of H in the same way, except that e_m stands for the edge pq. With respect to such ordering of edges, we have

$$A(L_G) - A(L_H) = \left[\begin{array}{c|c} 0 & a \\ \hline a^T & 0 \end{array}\right],$$

where $a = (a_1,\ldots,a_{m-1})^T$ is given by

$$a_s = \begin{cases} 1 & \text{if } e_s = uw,\ w \neq p, v, \\ -1 & \text{if } e_s = pw,\ w \neq u, v, \\ 0 & \text{otherwise.} \end{cases}$$

Since $r \geqslant 2$, G must contain a vertex different from u, v, p. So the vector a is nonzero. On the other hand, from the relation $(A(L_G) - A(L_H))y = 0$ we obtain $y_{m-1}a = 0$ and hence $a = 0$ as $y_{m-1} > 0$. So we arrive at a contradiction. This shows that we must have $\rho(A(L_G)) < \rho(A(L_H))$ and hence $\rho(Q(G)) < \rho(Q(H))$.

Case 2: $1 < i < \frac{r+1}{2}$. For convenience, we denote $r + 1 - i$ by j. In this case, we have

$$\sum_{e\in N_{L_H}(pq)} y_e = \sum_{w\in V(G)\setminus\{p\}} y_{pw} = \sum_{w\in V(G)\setminus\{p\}} (x_p + x_w) = (n-2)\xi_r + \sum_{w\in V(G)} x_w$$

and

$$\begin{aligned}\sum_{e\in N_{L_G(uv)}} y_e &= \sum_{w\in\cup_{k=i}^r V_k\setminus\{u,v\}} y_{uw} + \sum_{w\in\cup_{k=j}^r V_k\setminus\{u\}} y_{vw} \\ &= \left(\sum_{k=i}^r n_k - 4\right)x_u + \sum_{w\in\cup_{k=i}^r V_k} x_w + \left(\sum_{k=j}^r n_k - 2\right)x_v + \sum_{w\in\cup_{k=j}^r V_k} x_w.\end{aligned}$$

Thus,

$$\begin{aligned}
&\sum_{e\in N_{L_H}(pq)} y_e - \sum_{e\in N_{L_G}(uv)} y_e \\
&= (n-2)\xi_r + \sum_{w\in\cup_{k=1}^{i-1}V_k} x_w - \sum_{w\in\cup_{k=j}^{r}V_k} x_w - \left(\sum_{k=i}^{r} n_k - 4\right)\xi_j - \left(\sum_{k=j}^{r} n_k - 2\right)\xi_i \\
&= (n-2)\xi_r + \sum_{k=1}^{i-1} n_k\xi_k - \sum_{k=j}^{r} n_k\xi_k - (\delta_j - 3)\xi_j - (\delta_i - 2)\xi_i = z^T\xi,
\end{aligned}$$

where

$$z = (n_1,\ldots,n_{i-1}, \underset{\substack{\uparrow\\ i\text{th}}}{-(\delta_i-2)}, 0,\ldots,0, \underset{\substack{\uparrow\\ j\text{th}}}{-(\delta_j+n_j-3)}, -n_{j+1},\ldots,-n_{r-1}, \underset{\substack{\uparrow\\ r\text{th}}}{n-n_r-2})^T.$$

By a well-known lower bound for the signless Laplacian spectral radius (see, for instance, [14, Lemma B]), $\rho \geqslant d_{\max}(G)+1$; so we have $\rho-\delta_j > 0$. Since $z^T(B+\Delta-\delta_j I)\xi = (\rho-\delta_j)z^T\xi$, to prove that the right side of (3.1) is positive, it suffices to show that $z^T(B+\Delta-\delta_j I)\xi$ is positive. The latter quantity can be computed by considering the sum $\sum_{k=1}^{r}[z^T(B+\Delta-\delta_j I)]_k\xi_k$. Making use of the known relations between the n_i's and δ_i's (see (2.2) and (2.3)), we evaluate the components $[z^T(B+\Delta-\delta_j I)]_k$ by treating separately the cases $k=r, k=j+1,\ldots,r-1, k=j, k=i+1,\ldots,j-1, k=i, k=2,\ldots,i-1$ and $k=1$. After some tedious calculations the above expression becomes

$$\begin{aligned}
&[2n_r(n+1-\delta_j-\delta_i)+(n-n_r-2)(n-\delta_j-2)]\xi_r + (n+4-\delta_j-2\delta_i)\sum_{k=j+1}^{r-1} n_k\xi_k \\
&+ [n_j(n+4-\delta_j-2\delta_i)+(\delta_j-3)]\xi_j + (n+1-\delta_j-\delta_i)\sum_{k=i+1}^{j-1} n_k\xi_k \\
&+ [n_i(n+1-\delta_j-\delta_i)+(\delta_i-2)(\delta_j-\delta_i)]\xi_i + (n-2-\delta_j)\sum_{k=1}^{i-1} n_k\xi_k.
\end{aligned}$$

We claim that the above expression is positive. Once this is established, by (3.1) it will follow that $y^TA(L_H)y - y^TA(L_G)y > 0$, as desired.

Note that by our hypothesis, $\delta_j+\delta_i \leqslant n+1$ (recalling that $j=r+1-i$). Also, we have $n-1=\delta_r > \delta_j > \delta_i > \delta_1 = n_r \geqslant 1$ which implies $\delta_i \geqslant 2, \delta_j \geqslant 3, n-n_r-2 > 0$ and $n-2-\delta_j \geqslant 0$.

If $\delta_j+2\delta_i \leqslant n+3$, then clearly the said expression is positive. If $\delta_j+2\delta_i = n+4$, then the said expression is also positive because then we must have either $n+1 > \delta_i+\delta_j$ or $\delta_j > 3$ (as $\delta_j=3$, together with the inequalities $\delta_j > \delta_i > \delta_1 \geqslant 1$, implies $\delta_i = 2$).

If $\delta_j+2\delta_i > n+4$, then $\delta_i > n+4-\delta_i-\delta_j \geqslant 3$ and so $\delta_j > 3$. In this case, we can write the said expression as the sum of

$$[2n_r(n+1-\delta_j-\delta_i)+(n-n_r-2)(n-2-\delta_j)]\xi_r + (n+4-\delta_j-2\delta_i)\sum_{k=j}^{r-1} n_k\xi_k$$

and some nonnegative terms. A little calculation yields

$$\begin{aligned}
&2n_r(n+1-\delta_j-\delta_i)+(n-n_r-2)(n-2-\delta_j)+(n+4-\delta_j-2\delta_i)\sum_{k=j}^{r-1} n_k \\
&= (n+1-\delta_j-\delta_i)(n-2+\delta_i)+(\delta_i-3)(n-2-\delta_i) > 0.
\end{aligned}$$

Since $\xi_r > \xi_k$ for $k=j,\ldots,r-1$, we have

$$[2n_r(n+1-\delta_j-\delta_i)+(n-n_r-2)(n-2-\delta_j)]\xi_r+\sum_{k=j}^{r-1}n_k(n+4-\delta_j-2\delta_i)\xi_k>0$$

and so the said expression is positive.

Case 3: $i=\frac{r+1}{2}$ (with r odd). In this case, $\sum_{e\in N_{L_H}(pq)}y_e-\sum_{e\in N_{L_G}(uv)}y_e$ is equal to

$$\sum_{w\in V(G)\setminus\{p\}}(x_p+x_w)-\left[\sum_{w\in\cup_{k=i}^r V_k\setminus\{u,v\}}(x_u+x_w)+\sum_{w\in\cup_{k=i}^r V_k\setminus\{u,v\}}(x_v+x_w)\right],$$

or

$$\left[(n-2)\xi_r+\sum_{w\in V(G)}x_w\right]-2\left[\left(\sum_{k=i}^r n_k-4\right)\xi_i+\sum_{k=i}^r n_k\xi_k\right]$$

and after some calculations it becomes $z^T\xi$, where

$$z=(n_1,\ldots,n_{i-1},-(2\delta_i+n_i-6),-n_{i+1},\ldots,-n_{r-1},n-n_r-2)^T.$$

As for Case 2, we find $z^T\xi$ by looking at $z^T(B+\Delta-\delta_iI)\xi$ and calculate the latter by considering the sum $\sum_{k=1}^r[z^T(B+\Delta-\xi_iI)]_k\xi_k$. After some tedious calculations, the latter quantity becomes

$$[2n_r(n+1-2\delta_i)+(n-n_r-2)(n-2-\delta_i)]\xi_r+\sum_{k=i+1}^{r-1}n_k(n+4-3\delta_i)\xi_k$$
$$+[n_i(n+4-3\delta_i)+2(\delta_i-3)]\xi_i+\sum_{k=1}^{i-1}n_k(n-2-\delta_i).$$

Since $i=\frac{r+1}{2}$, by our hypothesis, $n+1\geqslant\delta_i+\delta_{r+1-i}=2\delta_i$. Note that $n-n_r-2>0$ as r is an odd integer at least 3, $n=\sum_{k=1}^r n_k$, $n_k\geqslant 1$ for each k and $n_{\lceil\frac{r}{2}\rceil}\geqslant 2$. Moreover, we also have $\delta_i\leqslant n-2$ and $n_i\geqslant 2$.

First, consider the case when $3\delta_i\leqslant n+4$. We can write the above expression as the sum of $(n+4-3\delta_i)\sum_{k=i}^{r-1}n_k\xi_k+(2\delta_i-6)\xi_i$ and some nonnegative terms. Now

$$(n+4-3\delta_i)\sum_{k=i}^{r-1}n_k\xi_k+(2\delta_i-6)\xi_i\geqslant[(n+4-3\delta_i)n_i+2\delta_i-6]\,\xi_i$$
$$=[(n_i-1)(n+4-3\delta_i)+(n-2-\delta_i)]\,\xi_i\geqslant 0$$

and we have

$$(n+4-3\delta_i)\sum_{k=i}^{r-1}n_k\xi_k+(2\delta_i-6)\xi_i=0$$

only if

$$n+4-3\delta_i=0\quad\text{and}\quad 2\delta_i-6=0.$$

The latter conditions imply that $\delta_i=3$ and $n=5$. Since r is an odd integer at least 3, we must have $r=3$ and $i=2$. Hence we have $G=C(1,2,2)$ or $C(1,3,1)$. The preceding argument, in fact, shows that when $3\delta_i\leqslant n+4$, the said expression is always positive except possibly when $G=C(1,2,2)$ or $C(1,3,1)$. (One can check that when G is equal to one of these two maximal graphs, the said expression is equal to zero, but we do not need this in our subsequent argument.)

It is known that for $n\geqslant 5$ there are precisely two tricyclic maximal graphs of order n and they have equal signless Laplacian spectral radius (see [23, Lemma 5.6 and the preceding discussion]). For $n=5$, the said pair of maximal graphs are $C(1, 3, 1)$ and $C(3, 2)$. Now $C(3, 2)$ is a maximal graph with precisely two dominating vertices and $C(2, 2, 1, 1)$ is the maximal graph obtained from $C(3, 2)$ by deleting an edge joining one dominating vertex to a vertex of least degree and adding one edge joining the other dominating vertex to a new vertex, by the already proved Case 1, $\rho(Q(C(3, 2))) < \rho(Q(C(2, 2, 1, 1)))$. So we have $\rho(Q(C(1, 3, 1))) < \rho(Q(C(2, 2, 1, 1)))$, and this is what we want, because $C(2, 2, 1, 1)$ is also equal to the maximal graph obtained from $C(1, 3, 1)$ by deleting an edge joining a pair of vertices belonging to the middle neighborhood equivalence class and adding an edge joining the dominating vertex to a new vertex.

We are also required to establish the inequality $\rho(Q(C(1, 2, 2))) < \rho(Q(C(1, 3, 1, 1)))$. For the purpose, we compare their reduced signless Laplacian spectral radii. By definition, we have

$$(\Delta + B)(C(1, 2, 2)) = \begin{bmatrix} 2 & 0 & 2 \\ 0 & 4 & 2 \\ 1 & 2 & 5 \end{bmatrix} \quad \text{and} \quad (\Delta + B)(C(1, 3, 1, 1)) = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 2 & 1 & 1 \\ 0 & 3 & 4 & 1 \\ 1 & 3 & 1 & 5 \end{bmatrix}.$$

After some calculations we obtain

$$q_{C(1,2,2)}(x) = x^3 - 11x^2 + 32x - 24,$$
$$q_{C(1,3,1,1)}(x) = x^4 - 12x^3 + 41x^2 - 42x + 12$$

and

$$q_{C(1,3,1,1)}(x) = (x - 1)q_{C(1,2,2)}(x) - 2(x - 1)(x - 6).$$

Denote $\rho(Q(C(1, 2, 2)))$ by ρ. Since $q_{C(1,2,2)}(6) = -12 < 0$, $\rho > 6$. So we have

$$q_{C(1,3,1,1)}(\rho) = -2(\rho - 6)(\rho - 1) < 0$$

and hence $\rho(Q(C(1, 2, 2))) < \rho(Q(C(1, 3, 1, 1)))$.

It remains to treat the case when $3\delta_i > n + 4$. Then $\frac{n+4}{3} < \delta_i \leqslant \frac{n+1}{2}$, which implies $n > 5$ and hence $\delta_i > \frac{n+4}{3} > 3$. So the said expression is greater than ξ_i times the following quantity

$$2n_r(n + 1 - 2\delta_i) + (n - n_r - 2)(n - 2 - \delta_i) + (n + 4 - 3\delta_i) \sum_{k=i}^{r-1} n_k.$$

Making use of the relation $\sum_{k=i}^{r} n_k = \delta_i + 1$ (as $i = \frac{r+1}{2}$), after some calculations, one can show that the latter quantity is equal to

$$(n + 1 - 2\delta_i)(n + \delta_i) + (\delta_i - 4)(n - 2 - \delta_i),$$

which is clearly nonnegative. So in this case the said expression is also positive. The proof is complete. □

One may ask whether it is possible to extend Theorem 3.6 somehow to cover the case $r = 1$. More specifically, if u, v, p are distinct vertices of K_n, is it true that $\rho(Q(K_n)) < \rho(Q(K_n - uv + pq))$, where q is a new vertex? For $n = 3$, the answer to the latter question is in the negative, because $K_3 - uv + pq = K_{1,3}$ and it is known that $\rho(Q(K_3)) = \rho(Q(K_{1,3}))$. For $n \geqslant 4$, the answer is also in the negative. In fact, the inequality goes the other way.

Remark 3.7. For every positive integer $n \geqslant 4$, $\rho(Q(K_n)) > \rho(Q(C(1, 2, n - 3, 1)))$.

Proof. By definition

$$(\Delta + B)(C(1, 2, n - 3, 1)) = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & n-2 & n-3 & 1 \\ 0 & 2 & 2n-5 & 1 \\ 1 & 2 & n-3 & n \end{bmatrix}.$$

A straightforward calculation yields

$$q_{C(1,2,n-3,1)}(x) = (x-2n+2)[x^3-(2n-4)x^2+(n^2-3n+1)x-(n^2-9n+18)] + 6n^2-22n+12.$$

Hence we have $q_{C(1,2,n-3,1)}(2n-2) = 6n^2-22n+12 > 0$ for $n \geqslant 4$. Since $q_{C(1,2,n-3,1)}(x)$ is positive for x sufficiently large, if $q_{C(1,2,n-3,1)}(x)$ has a root greater than $2n-2$, then (counting multiplicities) it must have at least two such roots and the sum of such roots is greater than $4n-4$, which contradicts the fact that $(\Delta+B)(C(1,2,n-3,1))$ is a positive definite matrix with trace equal to $4n-6$. So $q_{C(1,2,n-3,1)}(x)$ cannot have a root greater than $2n-2$. This proves that $\rho(Q(C(1,2,n-3,1))) < 2n-2 = \rho(Q(K_n))$. $\square$

Lemma 3.8. *Let G be a maximal graph with at least two neighborhood equivalence classes. Let u, v be a complementary pair of adjacent vertices, and let p, q be a complementary pair of nonadjacent vertices, each different from u, v. Assume that G has two or more dominating vertices if u or v is a dominating vertex. Then $G-uv+pq$ is a maximal graph.*

Proof. By Lemma 3.5, $G-uv$ is a maximal graph and p, q form a complementary pair of nonadjacent vertices of $G-uv$. By Remark 3.4 it follows that $G-uv+pq$ is a maximal graph. $\square$

Theorem 3.9. *Let G be a maximal graph with r neighborhood equivalence classes. Let $\delta_r > \delta_{r-1} > \cdots > \delta_1$ be the distinct vertex degrees of G. If there exist positive integers i, l with $l+2 \leqslant i \leqslant \left\lceil \frac{r}{2} \right\rceil$ such that $\delta_i + \delta_{r+1-i} \leqslant \delta_l + \delta_{r-l} + 1$, then $\rho(Q(G)) < \rho(Q(H))$ for some maximal graph H with the same number of vertices and edges as G.*

Proof. For convenience, denote $r+1-i$ by j. Take $u \in V_j$, $v \in V_i$, $p \in V_{r-l}$ and $q \in V_l$. By Lemma 3.8, $H := G-uv+pq$ is a maximal graph. We are going to show that $\rho(Q(G)) < \rho(Q(H))$. The argument is similar to that used in the proof for Theorem 3.6, but the calculation is more involved. Let $x, y, \xi_k (k = 1, \ldots, r)$, ξ and ρ have the same meanings as in the proof of Theorem 3.6. Then

$$y^T A(L_H)y - y^T A(L_G)y = 2y_{uv}\left[\sum_{e \in N_{L_H}(pq)} y_e - \sum_{e \in N_{L_G}(uv)} y_e\right]. \tag{3.2}$$

We first deal with the case when $\frac{r+1}{2} > i$. We have

$$\sum_{e \in N_{L_H}(pq)} y_e = \sum_{w \in N_H(p)\backslash\{q\}} (x_p + x_w) + \sum_{w \in N_H(q)\backslash\{p\}} (x_q + x_w)$$
$$= (\delta_{r-l}-1)\xi_{r-l} + \sum_{k=l+1}^{r} n_k\xi_k + \delta_l\xi_l + \sum_{k=r+1-l}^{r} n_k\xi_k$$

and a similar expression for $\sum_{e \in N_{L_G}(uv)} y_e$. After some calculations, we find that $\sum_{e \in N_{L_H}(pq)} y_e - \sum_{e \in N_{L_G}(uv)} y_e$ is equal to the following expression

$$(\delta_{r-l}-n_{r-l}-1)\xi_{r-l} + \sum_{k=l+1}^{i-1} n_k\xi_k + \delta_l\xi_l - (\delta_j+n_j-3)\xi_j - (\delta_i-2)\xi_i - \sum_{k=j+1}^{r-l-1} n_k\xi_k.$$

Since $j = r+1-i > i \geqslant l+2 \geqslant 3$, by (2.4) we have $\delta_i \geqslant i > 2$ and $\delta_j + n_j - 3 > 0$. As $\xi_{r-l} > \xi_k$ for $k \leqslant r-l-1$, the above expression is not less than ξ_{r-l} times $(\delta_{r-l}-n_{r-l}-1) - (\delta_j+n_j-3) - (\delta_i-2) - \sum_{k=j+1}^{r-l-1} n_k$. The latter quantity is, in turn, equal to $\delta_{r-l}+\delta_l-\delta_j-2\delta_i+4$. So $\sum_{e \in N_{L_H}(pq)} y_e - \sum_{e \in N_{L_G}(uv)} y_e$ is positive whenever $\delta_{r-l}+\delta_l-\delta_j-2\delta_i+4 \geqslant 0$. Hereafter, we assume that $\delta_j + 2\delta_i \geqslant \delta_{r-l}+\delta_l+5$.

Let $z \in \mathbb{R}^r$ denote the vector

$$(0, \ldots, 0, \underset{\substack{\uparrow \\ l\text{th}}}{\delta_l}, n_{l+1}, \ldots, \underset{\substack{\uparrow \\ (i-1)\text{th}}}{n_{i-1}}, -(\delta_i - 2), 0, \ldots, 0, -\underset{\substack{\uparrow \\ j\text{th}}}{(\delta_j + n_j - 3)},$$

$$-n_{j+1}, \ldots, -n_{r-l-1}, \delta_{r-l} - \underset{\substack{\uparrow \\ (r-l)\text{th}}}{n_{r-l}} - 1, 0, \ldots, \underset{\substack{\uparrow \\ r\text{th}}}{0})^T.$$

Then $\sum_{e \in N_{L_H}(pq)} y_e - \sum_{e \in N_{L_G}(uv)} y_e = z^T\xi$. Since $(\rho - \delta_j)z^T\xi = z^T(B + \Delta - \delta_j I)\xi$ and $\rho - \delta_j > 0$, it suffices to show that $z^T(B + \Delta - \delta_j I)\xi$ is positive. After some tedious calculations, we find that the latter quantity is equal to $\sum_{k=l}^{r} c_k\xi_k$, where

$$c_k = \begin{cases} 2n_k(\delta_{r-l} + \delta_l - \delta_j - \delta_i + 2) & k = r - l + 1, \ldots, r, \\ 2n_{r-l}(\delta_{r-l} + \delta_l - \delta_j - \delta_i + 2) & \\ \quad +(\delta_{r-l} - n_{r-l} - 1)(\delta_{r-l} - \delta_j - 1) - n_{r-l}\delta_l & k = r - l, \\ n_k(\delta_{r-l} + \delta_l - \delta_j - 2\delta_i + 5) & k = j + 1, \ldots, r - l - 1, \\ n_j(\delta_{r-l} + \delta_l - \delta_j - 2\delta_i + 5) + (\delta_j - 3) & k = j, \\ n_k(\delta_{r-l} + \delta_l - \delta_j - \delta_i + 2) & k = i + 1, \ldots, j - 1, \\ n_i(\delta_{r-l} + \delta_l - \delta_j - \delta_i + 2) + (\delta_i - 2)(\delta_j - \delta_i) & k = i, \\ n_k(\delta_{r-l} + \delta_l - \delta_j - 1) & k = l + 1, \ldots, i - 1, \\ -\delta_l(\delta_j - \delta_l) & k = l. \end{cases}$$

Note that $c_k > 0$ for $r - l + 1 \leqslant k \leqslant r$ and $l + 1 \leqslant k \leqslant j - 1$, and $c_k \leqslant 0$ for $j + 1 \leqslant k \leqslant r - l - 1$ and $k = l$. Since

$$\begin{aligned} &\sum_{k=j+1}^{r} c_k\xi_k + n_j(\delta_{r-l} + \delta_l - \delta_j - 2\delta_i + 5)\xi_j \\ &\quad \geqslant \sum_{k=j+1}^{r-l-1} c_k\xi_{r-l} + c_{r-l}\xi_{r-l} + \sum_{k=r-l+1}^{r} c_k\xi_{r-l} + n_j(\delta_{r-l} + \delta_l - \delta_j - \delta_i + 5)\xi_{r-l} \end{aligned}$$

and

$$\sum_{k=l}^{j-1} c_k\xi_k + (\delta_j - 3)\xi_j \geqslant c_l\xi_l + \sum_{l=l+1}^{j-1} c_k\xi_l + (\delta_j - 3)\xi_l$$

in order to have $\sum_{k=l}^{r} c_k\xi_k > 0$, it suffices to show that

$$\sum_{k=j+1}^{r} c_k + n_j(\delta_{r-l} + \delta_l - \delta_j - 2\delta_i + 5) > 0 \quad \text{and} \quad (\delta_j - 3) + \sum_{k=l}^{j-1} c_k > 0.$$

By calculation we have

$$\begin{aligned} &\sum_{k=j+1}^{r} c_k + n_j(\delta_{r-l} + \delta_l - \delta_j - 2\delta_i + 5) \\ &\quad = (\delta_{r-l} + \delta_l - \delta_j - \delta_i + 1)(\delta_i + \delta_l + \delta_{r-l} - 1) \\ &\qquad + 2n_{r-l} + 2(\delta_i - \delta_{l+1}) + (\delta_{r-l} - \delta_i - 1)(\delta_i - \delta_l - 2), \end{aligned}$$

and

$$\begin{aligned} (\delta_j - 3) + \sum_{k=l}^{j-1} c_k &= (\delta_{r-l} + \delta_l - \delta_j - \delta_i + 1)(\delta_{r-l} + \delta_l - \delta_i + 1) \\ &\quad + (\delta_{r-l} - \delta_i)(\delta_i - \delta_l - 2) + 2\delta_j - \delta_i - \delta_l - 2. \end{aligned}$$

So the two desired inequalities both hold.

Now we treat the remaining case when $i = \frac{r+1}{2}$ (with odd r). In this case, $r + 1 - i = i$ and after some calculations we obtain

$$\sum_{e \in N_{L_H}(pq)} y_e - \sum_{e \in N_{L_G}(uv)} y_e$$
$$= (\delta_{r-l} - n_{r-l} - 1)\xi_{r-l} + \sum_{k=l+1}^{i-1} n_k\xi_k + \delta_l\xi_l - (2\delta_i + n_i - 6)\xi_i - \sum_{k=i+1}^{r-l-1} n_k\xi_k.$$

Note that $2\delta_i + n_i - 6 > 0$ as $\delta_i \geqslant 3$, and

$$(\delta_{r-l} - n_{r-l} - 1) - (2\delta_i + n_i - 6) - \sum_{k=i+1}^{r-l-1} n_k = \delta_l + \delta_{r-l} - 3\delta_i + 4.$$

If $3\delta_i \leqslant \delta_l + \delta_{r-l} + 4$ then clearly $\sum_{e \in N_{L_H}(pq)} y_e - \sum_{e \in N_{L_G}(uv)} y_e > 0$. Hereafter, we assume that $3\delta_i \geqslant \delta_l + \delta_{r-l} + 5$ (and $2\delta_i < \delta_l + \delta_{r-l} + 2$). Let z denote the vector

$$(0, \ldots, 0, \underset{\substack{\uparrow \\ l\text{th}}}{\delta_l}, n_{l+1}, \ldots, n_{i-1}, \underset{\substack{\uparrow \\ i\text{th}}}{-(2\delta_i + n_i - 6)}, -n_{i+1}, \ldots, -n_{r-l-1}, \underset{\substack{\uparrow \\ (r-l)\text{th}}}{\delta_{r-l} - n_{r-l} - 1}, 0, \ldots, \underset{\substack{\uparrow \\ r\text{th}}}{0})^T.$$

Then $\sum_{e \in N_{L_H}(pq)} y_e - \sum_{e \in N_{L_G}(uv)} y_e = z^T\xi$. Again it suffices to show that $z^T(B + \Delta - \delta_i I)\xi$ is positive. After some tedious calculations the latter quantity becomes $\sum_{k=l}^{r} c_k\xi_k$, where

$$c_k = \begin{cases} 2n_k(\delta_{r-l} + \delta_l - 2\delta_i + 2) & k = r - l + 1, \ldots, r, \\ 2n_{r-l}(\delta_{r-l} + \delta_l - 2\delta_i + 2) & \\ \quad +(\delta_{r-l} - n_{r-l} - 1)(\delta_{r-l} - \delta_i - 1) - n_{r-l}\delta_l & k = r - l, \\ n_k(\delta_{r-l} + \delta_l - 3\delta_i + 5) & k = i + 1, \ldots, r - l - 1, \\ n_i(\delta_{r-l} + \delta_l - 3\delta_i + 5) + 2\delta_i - 6 & k = i, \\ n_k(\delta_{r-l} + \delta_l - \delta_i - 1) & k = l + 1, \ldots, i - 1, \\ -\delta_l(\delta_i - \delta_l) & k = l. \end{cases}$$

Note that $c_k > 0$ for $r - l + 1 \leqslant k \leqslant r$ and $l + 1 \leqslant k \leqslant i - 1$, and $c_k \leqslant 0$ for $i + 1 \leqslant k \leqslant r - l - 1$ and $k = l$. In order to have $\sum_{k=l}^{r} c_k\xi_k > 0$, it suffices to show that

$$\sum_{k=i+1}^{r} c_k, \; \sum_{k=i+1}^{r} c_k + n_i(\delta_{r-l} + \delta_l - 3\delta_i + 5) + (\delta_i - 6) \quad \text{and} \quad \delta_i + \sum_{k=l}^{i-1} c_k$$

are all positive quantities. Now by calculation we have

$$\sum_{k=i+1}^{r} c_k = (\delta_{r-l} + \delta_l - 2\delta_i + 1)(\delta_{r-l} + \delta_l + \delta_{i-1} - 1)$$
$$+(\delta_{r-l} - \delta_{i-1} - 1)(\delta_i - \delta_l - 2) + \delta_l(n_i - 1) + 2(\delta_{i-1} - \delta_l),$$
$$\sum_{k=i+1}^{r} c_k + n_i(\delta_{r-l} + \delta_l - 3\delta_i + 5) + (\delta_i - 6)$$
$$= (\delta_{r-l} + \delta_l - 2\delta_i + 1)(\delta_{r-l} + \delta_l + \delta_i) + (\delta_i - \delta_l - 2)(\delta_{r-l} - \delta_i + 1) + 2$$

and

$$\delta_i + \sum_{k=l}^{i-1} c_k = (\delta_{r-l} + \delta_l - 2\delta_i + 1)(\delta_{r-l} + \delta_l - \delta_i) + (\delta_i - \delta_l - 2)(\delta_{r-l} - \delta_i + 1) + 2.$$

So it is clear that the three said quantities are all positive. The proof is complete. $\square$

We call a connected graph *signless Laplacian maximizing* if it maximizes the signless Laplacian spectral radius over all connected graphs with given numbers of vertices and edges. According to Lemma 2.2, every signless Laplacian maximizing graph is a (degree) maximal graph.

By Theorem 3.9 we immediately obtain a set of conditions necessary for a maximal graph to be signless Laplacian maximizing:

Theorem 3.10. *Let G be a signless Laplacian maximizing graph with n vertices and $r(\geqslant 5)$ neighborhood equivalence classes. Let $\delta_r > \delta_{r-1} > \cdots > \delta_1$ be the distinct vertex-degrees of G. Then $\delta_i + \delta_{r+1-i} \geqslant \delta_l + \delta_{r-l} + 2$ for every pair of positive integers i, l that satisfy $l + 2 \leqslant i \leqslant \left\lceil \frac{r}{2} \right\rceil$.*

Corollary 3.11. *If G is a signless Laplacian maximizing graph with n vertices and r neighborhood equivalence classes then $r \leqslant \frac{4}{5}n$.*

Proof. The necessary condition for a signless Laplacian maximizing graph as given in Theorem 3.10 can be rewritten as $\delta_i - \delta_l \geqslant \delta_{r-l} - \delta_{r+1-i} + 2$, whenever i, l are positive integers that satisfy $l + 2 \leqslant i \leqslant \left\lceil \frac{r}{2} \right\rceil$. Note that $\delta_{r-l} - \delta_{r+1-i} \geqslant 1$ as $(r-l) - (r+1-i) = i - (l+1) \geqslant 1$. So $\delta_i \geqslant \delta_l + 3$ whenever $i \geqslant l + 2$. Hence, for every pair of positive integers i, j with $j \leqslant i \leqslant \left\lceil \frac{r}{2} \right\rceil$, $i - j = 2k$, we have $\delta_i \geqslant \delta_j + 3k$.

Write r as $4k + s$, where k is a nonnegative integer and s is a positive integer not greater than 4. We have

$$\delta_{\lceil \frac{r}{2} \rceil} \geqslant \delta_1 + 3k \geqslant 3k + 1 \quad \text{if } s = 1, 2,$$

and

$$\delta_{\lceil \frac{r}{2} \rceil} \geqslant \delta_2 + 3k \geqslant 3k + 2 \quad \text{if } s = 3, 4.$$

When $s = 2, 4$ (i.e., when r is even), we have

$$n - 1 = \delta_r = \delta_{\lceil \frac{r}{2} \rceil} + n_{\lceil \frac{r}{2} \rceil} + \cdots + n_1 - 1 \geqslant \delta_{\lceil \frac{r}{2} \rceil} + \left\lceil \frac{r}{2} \right\rceil.$$

When $s = 1, 3$, we have

$$n - 1 = \delta_r = \delta_{\lceil \frac{r}{2} \rceil} + n_{\lceil \frac{r}{2} \rceil - 1} + \cdots + n_1 \geqslant \delta_{\lceil \frac{r}{2} \rceil} + \left\lceil \frac{r}{2} \right\rceil - 1.$$

Noting that

$$\left\lceil \frac{r}{2} \right\rceil = \begin{cases} 2k + 1 & \text{if } s = 1, 2, \\ 2k + 2 & \text{if } s = 3, 4 \end{cases}$$

and making use of the above inequalities, we obtain

$$n - 1 \geqslant 5k + s = \frac{5}{4}(r - s) + s.$$

Rewriting the preceding inequality, we have

$$r \leqslant \frac{4}{5}(n - s - 1) + s = \frac{4}{5}n - \frac{1}{5}(4 - s) \leqslant \frac{4}{5}n. \quad \square$$

It is worth noting that in [24, Theorem 6.3] the following necessary condition is also obtained for a signless Laplacian maximizing graph with distinct vertex-degrees $\delta_r > \delta_{r-1} > \cdots > \delta_1$:

$$\delta_l + \delta_{r-l} + 1 \leqslant \delta_{k+1} + \delta_{r-k}$$

for every pair of positive integers k, l that satisfy $l < k \leqslant \left\lfloor \frac{r}{2} \right\rfloor - 1$. By setting $i = k + 1$, one can readily see that the latter result is weaker than our Theorem 3.10. We obtain a stronger result at the expense of a much longer and harder proof.

For completeness, before we end this section we would like to consider the question of whether it is possible that for a maximal graph G there exist an edge uv and a pair of nonadjacent vertices p, q such that $G - uv + pq$ is a maximal graph but it is not true that u, v is a complementary pair of adjacent vertices and p, q is a complementary pair of nonadjacent vertices.

We begin with the situation when u, v do not form a complementary pair of adjacent vertices. Can we find a pair of nonadjacent vertices p, q of G such that $G - uv + pq$ is a maximal graph? To be specific, let $u \in V_i, v \in V_j$ with $i \leqslant j$.

First, we consider the case when $i + j > r + 2$. Take any vertex $p \in V_{j-2}$. We are going to show that p, v form a non-comparable pair of vertices of $G - uv$ with respect to its vicinal pre-order. Note that $v \not\geqslant^{G-uv} p$ because in the graph $G - uv$, u is adjacent to p (as $i + (j - 2) \geqslant r + 1$) but not adjacent to v. On the other hand, if we take any vertex $w \in V_{r+1-j} \cup V_{r+2-j}$ then w is adjacent to v in G and hence also in $G - uv$, whereas w is not adjacent to p in G nor in $G - uv$. So $p \not\geqslant^{G-uv} v$. The fact that v is not greater than or equal to p with respect to the vicinal pre-order clearly cannot be altered by the addition of an edge (different from uv) to $G - uv$. Since $V_{r+1-j} \cup V_{r+2-j}$ has cardinality at least two, we cannot make p greater than or equal to v with respect to the vicinal pre-order by the addition of one edge to $G - uv$. This disposes of the case when $i + j > r + 2$.

Now consider the case $i + j = r + 2$. Take any vertex $p \in V_{j-1}$ and apply a similar argument. We have $v \not\geqslant^{G-uv} p$ and $p \not\geqslant^{G-uv} v$. Again the former inequality cannot be altered by the addition of an edge to $G - uv$. If $|V_{r+1-j}| > 1$, then the latter inequality also cannot be altered. If, however, V_{r+1-j} is a singleton, say $\{q\}$, then by adding the edge pq to $G - uv$, we obtain $p \geqslant^{G-uv+pq} v$. Note that our preceding argument applies to an arbitrary vertex p of V_{j-1}. If V_{j-1} has more than one vertex, then clearly we cannot make the vicinal pre-order total by adding one edge to $G - uv$. So it remains to consider the case when $i + j = r + 2$ and V_{r+1-j}, V_{j-1} are both singletons, say $V_{j-1} = \{p\}$ and $V_{r+1-j} = \{q\}$. One can check that in this case the graphs G and $G - uv + pq$ share the same neighborhood equivalence classes except that q is interchanged with u and p is interchanged with v. So the graphs are isomorphic.

A moment's thought shows that the above argument in fact establishes the following:

Remark 3.12. Let G be a maximal graph with neighborhood equivalence classes $V_1, \ldots, V_r$. Let $u \in V_i, v \in V_j$ such that $i + j \geqslant r + 2$. Then for any pair of nonadjacent vertices p, q of G, the graph $G - uv + pq$ is not maximal, unless $i + j = r + 2$, V_{i-1}, V_{j-1} are both singletons and $V_{i-1} \cup V_{j-1} = \{p, q\}$, in which case $G - uv + pq$ is isomorphic with G.

Note that $G - uv + pq$ is the same as $G + pq - uv$. In a similar way, we can also establish the following:

Remark 3.13. Let G be a maximal graph with neighborhood equivalence classes $V_1, \ldots, V_r$. Let $p \in V_i, q \in V_j$ such that $i + j < r$. Then for any pair of adjacent vertices u, v of G, the graph $G - uv + pq$ is not maximal, unless $i + j = r - 1$, V_{i+1}, V_{j+1} are both singletons and $V_{i+1} \cup V_{j+1} = \{u, v\}$, in which case $G - uv + pq$ is isomorphic with G.

Remark 3.14. Let G be a maximal graph with neighborhood equivalence classes $V_1, \ldots, V_r$. Let $p \in V_i$ and let q be a new vertex. Then for any pair of adjacent vertices u, v of G, the graph $G - uv + pq$ is not threshold, unless $i = r - 1$, V_r, V_1 are singletons and $V_r \cup V_1 = \{u, v\}$, in which case $G - uv + pq$ is isomorphic with the threshold graph $G \cup K_1$.

4. Graphs with maximal signless Laplacian spectral radius

In this section we consider the problem of maximizing the signless Laplacian spectral radius over all connected graphs with m edges and at most $m - k$ vertices, where k is a given positive integer. Note that this is equivalent to the problem of maximizing the signless Laplacian spectral radius over all (not necessarily connected) graphs with m edges and $m - k$ vertices. Let us take a quick look at what have been done so far on this problem.

Rowlinson [21] has shown that for every pair of positive integers n, m with $n - 1 \leqslant m \leqslant \binom{n}{2}$ there is a unique graph with n vertices and m edges that maximizes the adjacency spectral radius among all graphs with n vertices and m edges, namely, the graph obtained in the following way: Write m as $\binom{d}{2} + t$, where $0 \leqslant t < d$, add a new vertex of degree t to the complete graph K_d and then take union with the null graph K^c_{n-d-1}. In [23], it is conjectured that the same graph also maximizes the signless Laplacian spectral radius among all graphs with n vertices and m edges, and also the nontrivial component of any other optimal graph must be of the same order. It turns out that the conjecture is far from being true (see [6]). In [6] the following is also established:

Remark 4.1. For every pair of positive integers m, n with $m \geqslant 4$, $n \geqslant m + 1$, the graph $K_{1,m+1} \cup K^c_{n-m-1}$ is the unique graph with n vertices and m edges that maximizes the signless Laplacian spectral radius among all graphs with n vertices and m edges.

In this section we treat the problem of determining graphs that maximize the signless Laplacian spectral radius over all graphs with m edges and $m - k$ vertices for $k = 0, 1, 2, 3$.

In [14, Lemma 1] the following observation was made:

Lemma 4.2. *Let G be a connected graph with n vertices and m edges such that $m - n + 1 = p$, $1 \leqslant p \leqslant \frac{(n-1)(n-2)}{2}$. If G is signless Laplacian maximizing, then the quantity* $\max\{d(u) + d(v) : uv \in E(G)\}$ *takes one of the values $n + 1, n + 2, \ldots, n + p$.*

The purpose of [14] is to characterize graphs that maximize the signless Laplacian spectral radius over all bicyclic graphs (i.e., connected graphs for which the number of edges is greater than the number of vertices by one). At the time when the research on [14] was carried out, it was not known that every signless Laplacian maximizing graph is a maximal graph. The preceding lemma has helped to narrow down the possible candidates for the signless Laplacian maximizing bicyclic graphs. It suffices to consider bicyclic graphs G for which the quantity $\max\{d(u) + d(v) : uv \in E(G)\}$ takes the value $n + 1$ or $n + 2$. For $n \geqslant 5$, there are nine possible candidates. After lengthy comparison, it turns out that the maximal graph $C(n - 4, 2, 1, 1)$ is the only bicyclic graph which is signless Laplacian maximizing. Of course, this is not a surprise now, because every signless Laplacian maximizing graph is maximal and there is (up to isomorphism) only one bicyclic maximal graph of a given order.

In this work, to search for threshold graphs (and, in particular, maximal graphs) that maximize the signless Laplacian spectral radius over a given class of graphs we also consider the possible values of $\max\{d(u) + d(v) : uv \in E(G)\}$ in our investigation, but we look at it from the viewpoint of the line graph of G. Note that if uv is an edge of G, then uv is incident with $d(u) - 1$ edges of G at u and $d(v) - 1$ edges at v, and so $d_{L_G}(uv) = d(u) + d(v) - 2$. Thus we have

$$\max\{d(p) + d(q) : pq \in E(G)\} = m + 1 - k \text{ if and only if } \max_{pq \in E(G)} d_{L_G}(pq) = m - 1 - k.$$

Moreover, any edge that attains the maximum is incident with every other edge of G except for k of them.

It should be added that when G is a graph with n vertices and m edges, the quantity $\max\{d(u) + d(v) : uv \in E(G)\}$ is bounded above by $\min\{2n - 2, m + 1\}$ as $d_{\max}(G) \leqslant n-1$ and $d_{\max}(L_G) \leqslant m-1$.

Lemma 4.3. *Let G be a maximal graph with m edges, different from K_1. Let k be a given nonnegative integer. The following conditions are equivalent:*

(a) $\max\{d(p) + d(q) : pq \in E(G)\} = m + 1 - k$.
(b) *G can be expressed as*

$$(((H \cup K^c_b) \vee K_1) \cup K^c_a) \vee K_1,$$

where a, b are nonnegative integers and H is a maximal graph with k edges, and in case $k = 0$, H can be the empty graph.

(c) *G is equal to one of the following graphs or is of one of the following forms:* K_n $\left(n \geqslant 2, k = \binom{n-2}{2}\right)$, $K_{1,m}$ *(for* $k = 0$*),* $C(n_1, n_2, p_1, \ldots, p_s, 1, 1)$ *(for* $k \geqslant 1$*),* $C(n_1, n_2, 1, 1)$ *(with* $n_2 \geqslant 2$*, for* $k = 0$*),* $C(n_1, p_1, \ldots, p_{s-1}, p_s + 1, 1)$ *(with* $s \geqslant 2$*),* $C(n_1, p_1 + 1, 1)$ $\left(\text{with } \binom{p_1}{2} = k\right)$, $C(n_1, p_1, \ldots, p_s, 2)$ *(for* $k \geqslant 1$*),* $C(n_1, 2)$ *(with* $n_1 \geqslant 2$*, for* $k = 0$*),* $C(p_1, \ldots, p_{s-1}, p_s + 2)$ *(with* $s \geqslant 2$*), where* $s, n_1, n_2, p_1, \ldots, p_s$ *are positive integers such that* $C(p_1, \ldots, p_s)$ *is a maximal graph with k edges.*

Proof. Let r denote the number of neighborhood equivalence classes of G.

(a) $\Rightarrow$ (c): Suppose that $\max\{d(p) + d(q) : pq \in E(G)\} = m + 1 - k$. Let $e = uv$ be an edge that attains the maximum. First, consider the case when G has precisely one dominating vertex. From the structure of a maximal graph, it is clear that one end vertex of e, say u, is a dominating vertex and the other end vertex, say v, is a vertex with the second largest distinct vertex degree. The graph $\widehat{G}$ obtained from G by removing u and all edges incident with u, together with all vertices of degree 1 (if any), is the empty graph if $r = 1$ or 2 and is a maximal graph if $r \geqslant 3$. In the former case, G equals K_n $\left(\text{with } m = \binom{n}{2} \text{ and } k = \binom{n-2}{2}\right)$ or is $K_{1,m}$ (with $k = 0$). Hereafter, we assume that $r \geqslant 3$. Then v is a dominating vertex of $\widehat{G}$ and $\widehat{G} \neq K_1$.

If v is the only vertex in G with the second largest distinct vertex degree, and hence the only dominating vertex of $\widehat{G}$, then the graph obtained from $\widehat{G}$ by removing v and all edges in $\widehat{G}$ incident with v, together with all vertices with degree 1 in $\widehat{G}$ – there is at least one vertex of degree 1, else $\widehat{G}$ is a complete graph with more than one vertex, in contradiction with the fact that v is the only dominating vertex of $\widehat{G}$ – is the empty graph when $k = 0$ and is a maximal graph with k edges when $k \geqslant 1$, say, it is $C(p_1, \ldots, p_s)$ where $s \geqslant 1$ (and with $p_1 \geqslant 2$ in case $s = 1$). If G has n_1 pendant vertices and $\widehat{G}$ has n_2 pendant vertices, then G equals $C(n_1, n_2, p_1, \ldots, p_s, 1, 1)$ (and equals $C(n_1, n_2, 1, 1)$ in case $k = 0$).

If G has more than one vertex with the second largest vertex degree, then the graph obtained from $\widehat{G}$ by removing v and all the edges incident with v is a maximal graph with k edges. In that case G is of the form $C(n_1, p_1, \ldots, p_{s-1}, p_s + 1, 1)$, where $s \geqslant 2, n_1, p_1, \ldots, p_s$ are positive integers such that $C(p_1, \ldots, p_s)$ is a maximal graph with k edges, or of the form $C(n_1, p_1 + 1, 1)$ with $\binom{p_1}{2} = k$ (which becomes $C(n_1, 2, 1)$ when $k = 0$).

Now we consider the case when G has two or more dominating vertices. Then the two end vertices of e must both be dominating vertices. If G has exactly two dominating vertices, then the graph obtained from G by removing u, v, all edges incident with u, v, and all vertices with degree 1 (if any) is a maximal graph with k edges and possibly the empty graph in case $k = 0$. So G is equal to K_2 or of the form $C(n_1, 2)$ (with $n_1 \geqslant 2$) when $k = 0$, and when $k \geqslant 1$ it is of the form $C(n_1, p_1, \ldots, p_s, 2)$, where $C(p_1, \ldots, p_s)$ is a maximal graph with k edges. If G has more than two dominating vertices, then the graph obtained from G by removing u, v and all edges incident with u, v is a maximal graph with k edges. In this case, G is equal to K_n (with $n \geqslant 3$) or is of the form $C(p_1, \ldots, p_{s-1}, p_s + 2)$ (which becomes K_{p_1+2} in case $s = 1$), where $C(p_1, \ldots, p_{s-1}, p_s)$ is a maximal graph with k edges.

(b) $\Rightarrow$ (c): Suppose $G = (((H \cup K_b^c) \vee K_1) \cup K_a^c) \vee K_1$. For $k \geqslant 1$, let $H = C(p_1, \ldots, p_s)$, where $s \geqslant 1$ (and $p_1 \geqslant 2$ if $s = 1$).

We have

$$G = \begin{cases} C(a, b, p_1, \ldots, p_s, 1, 1) & \text{when } a, b \geqslant 1, \\ C(a, p_1, \ldots, p_{s-1}, p_s + 1, 1) & \text{when } s \geqslant 2,\ a \geqslant 1,\ b = 0, \\ C(a, p_1 + 1, 1) & \text{when } s = 1,\ a \geqslant 1,\ b = 0, \\ C(b, p_1, \ldots, p_s, 2) & \text{when } a = 0,\ b \geqslant 1, \\ C(p_1, \ldots, p_{s-1}, p_s + 2) & \text{when } s \geqslant 2,\ a = b = 0, \\ K_n (n \geqslant 4) & \text{when } s = 1,\ a = b = 0. \end{cases}$$

If H is the empty graph K_0, then we have

$$G = \begin{cases} C(a,b,1,1) & \text{when } a \geqslant 1,\ b \geqslant 2,\\ C(a,2,1) & \text{when } a \geqslant 1,\ b = 1,\\ C(b,2) & \text{when } a = 0,\ b \geqslant 2,\\ K_3 & \text{when } a = 0,\ b = 1,\\ K_2 & \text{when } a = b = 0. \end{cases}$$

In any case, G is of one of the forms as given in (c).

(c) $\Rightarrow$ (b): Each of the maximal graphs $C(n_1, n_2, p_1, \ldots, p_s, 1, 1)$, $C(n_1, p_1, \ldots, p_{s-1}, p_s + 1, 1)$, $C(n_1, p_1, \ldots, p_s, 2)$ and $C(p_1, \ldots, p_{s-1}, p_s + 2)$ can be shown to be of the form as given in (b) by taking $H = C(p_1, \ldots, p_s)$ and (a, b) to be respectively (n_1, n_2), $(n_1, 0)$, $(1, n_1)$, $(0, 0)$. That the remaining maximal graphs listed in condition (c) are also of the form given in condition (b) is clear from the proof of (b) $\Rightarrow$ (c).

(b) $\Rightarrow$ (a): Suppose that G is of the form $(((H \cup K_b^c) \vee K_1) \cup K_a^c) \vee K_1$, where a, b are nonnegative integers. By definition of the join of two graphs, the two K_1's that appear in the representation of G are supposed to be different copies of the one-vertex graph. Denote by u the vertex for the outer K_1 and by v the vertex for the inner K_1. Clearly u is a dominating vertex of G. If $a = 0$, then v is also a dominating vertex of G. If $a > 0$ then u is the only dominating vertex of G and v is a vertex with the second largest vertex degree. In any case uv is an edge of G that attains the maximum value of $\max\{d(p) + d(q) : pq \in E(G)\}$. It is also readily seen that the edge uv is incident with every edge of G except for the k edges of H. It follows that

$$\max\{d(p) + d(q) : pq \in E(G)\} = d(u) + d(v) = m + 1 - k. \quad \square$$

Part (v) and (vi) of the following result are not needed in the subsequent parts of the paper.

Corollary 4.4. *Let G be a maximal graph with m edges. Then:*

(i) $\max\{d(u) + d(v) : uv \in E(G)\} = m + 1$ *if and only if G is of one of the following forms:* $C(n_1, n_2, 1, 1)$, $C(n_1, 1)$, $C(n_1, 2, 1)$, $C(n_1, 2)$, K_2 *or* K_3, *where n_1, n_2 are positive integers with $n_2 \geqslant 2$.*

(ii) $\max\{d(u) + d(v) : uv \in E(G)\} = m$ *if and only if G is of one of the following forms:* $C(n_1, n_2, 2, 1, 1)$, $C(n_1, 3, 1)$, $C(n_1, 2, 2)$ *or* K_4.

(iii) $\max\{d(u) + d(v) : uv \in E(G)\} = m - 1$ *if and only if G is of one of the following forms:* $C(n_1, n_2, 2, 1, 1, 1)$, $C(n_1, 2, 2, 1)$, $C(n_1, 2, 1, 2)$ *or* $C(2, 3)$.

(iv) $\max\{d(u) + d(v) : uv \in E(G)\} = m - 2$ *if and only if G is of one of the following forms:* $C(n_1, n_2, 3, 1, 1, 1)$, $C(n_1, n_2, 3, 1, 1)$, $C(n_1, 3, 2, 1)$, $C(n_1, 4, 1)$, $C(n_1, 3, 1, 2)$, $C(n_1, 3, 2)$, $C(3, 3)$ *or* K_5.

(v) $\max\{d(u) + d(v) : uv \in E(G)\} = m - 3$ *if and only if G is of one of the following forms:* $C(n_1, n_2, 1, 2, 1, 1, 1)$, $C(n_1, n_2, 4, 1, 1, 1)$, $C(n_1, 1, 2, 2, 1)$, $C(n_1, 1, 2, 1, 2)$, $C(n_1, 4, 2, 1)$, $C(n_1, 4, 1, 2)$, $C(1, 2, 3)$ *or* $C(4, 3)$.

(vi) $\max\{d(u) + d(v) : uv \in E(G)\} = m - 4$ *if and only if G is of one of the following forms:* $C(n_1, n_2, 2, 2, 1, 1, 1)$, $C(n_1, n_2, 5, 1, 1, 1)$, $C(n_1, n_2, 2, 2, 1, 1)$, $C(n_1, 2, 2, 2, 1)$, $C(n_1, 2, 2, 1, 2)$, $C(n_1, 5, 2, 1)$, $C(n_1, 2, 3, 1)$, $C(n_1, 5, 1, 2)$, $C(n_1, 2, 2, 2)$, $C(2, 2, 3)$, $C(5, 3)$ *or* $C(2, 4)$.

Proof. It is readily checked that K_1 (respectively, K_2, $C(2, 1)$) is the only maximal graph with no edge (respectively, one, two) edge(s), whereas there are two maximal graphs with three (respectively, four) edges, namely, $C(3, 1)$, K_3 (respectively, $C(4, 1)$, $C(1, 2, 1)$) and three maximal graphs with five edges, namely, $C(5, 1)$, $C(2, 2, 1)$, $C(2, 2)$. Parts (i)–(vi) of our result follows from Lemma 4.3 by taking k to be respectively $0, \ldots, 5$. As an illustration, we consider the proof for the part (iv). By Lemma 4.3, (a) $\Rightarrow$ (c), if G satisfies $\max\{d(p) + d(q) : pq \in E(G)\} = m + 1 - k$, then G is of one of the forms as given in condition (c). In particular, G can be of the form $C(n_1, p_1, \ldots, p_s, 2)$ or $C(p_1, \ldots, p_{s-1}, p_s + 2)$, where $C(p_1, \ldots, p_s)$ stands for a maximal graph with three edges; for graphs of the former kind there is no restriction on s, but for the second kind it is required that $s \geqslant 2$. Now there are precisely two maximal graphs with three edges, namely, $C(3)(= K_3)$ and $C(3, 1)(= K_{1,3})$. This leads to the following three possible forms for G: $C(n_1, 3, 1, 2)$, $C(n_1, 3, 2)$ and $C(3, 3)$. These graphs are listed in (iv). Conversely, suppose that G is a maximal graph with m edges and of the form $C(n_1, 3, 1, 2)$. Then since $C(3, 1)$ is a maximal graph with 3 edges, by Lemma 4.3, (c) $\Rightarrow$ (a), G satisfies $\max\{d(p) + d(q) : pq \in E(G)\} = m - 2$, as desired. $\square$

To find maximal graphs with m edges that satisfies $\max\{d(u) + d(v) : uv \in E(G)\} = m + 1 - k$ (for $k = 0, \ldots, 5$) we can apply Corollary 4.4. For instance, for $k = 5$, we consider the graphs listed in part (vi). Graphs of the form $C(n_1, n_2, 5, 1, 1, 1)$, where n_1, n_2 are positive integers, is a possible candidate. To find for the right pair (n_1, n_2), we solve the diophantine equation $m = |E(C(n_1, n_2, 5, 1, 1, 1)|$, i.e., $m = n_1 + 2n_2 + 18$. Depending on m, the diophantine equation may have no solution, one solution, or more than one solution. If, we look for maximal graphs not only with m edges but also with n vertices, then we have to consider also the condition $n = |V(G)|$, which is $n = n_1 + n_2 + 8$ in this case.

Now let us explain how the quantity $\max\{d(p) + d(q) : pq \in E(G)\}$ can play a role in searching for maximal graphs that maximize the signless Laplacian spectral radius over graphs with m edges and at most $m - k$ vertices. Let G_0 be a connected graph with m edges and at most $m - k$ vertices, which is an optimal graph for the problem. Choose a maximal graph H with m edges and $m - k$ vertices. By the known bounds for the signless Laplacian spectral radius of a graph (see [14, Lemma B]), we have

$$\max\{d(p) + d(q) : pq \in E(G_0)\} \geqslant \rho(Q(G_0)) \geqslant \rho(Q(H)) \geqslant d_{\max}(H) + 1 = m - k,$$

where the rightmost inequality is strict, unless H is regular or semi-regular. Now the complete graphs are the only regular maximal graphs and the stars $K_{1,p}$ are the only semi-regular maximal graphs. It is clear that when m is of the form $\binom{a}{2}$ for some positive integer $a \geqslant 2$ and $k = \binom{a-1}{2} - 1$ then K_a is the only maximal graph with m edges and $m - k(= a)$ vertices and there is no maximal graph with m edges and less than $m - k$ vertices – for such pair of m, k, the problem of maximizing the signless Laplacian spectral radius over all graphs with m edges and at most $m - k$ vertices is trivial. It is also readily seen that for nonnegative integer k there does not exist a semi-regular maximal graph with m edges and $m - k$ vertices. Thus, we have the following

Remark 4.5. If G_0 is a connected graph that maximizes the signless Laplacian spectral radius over all graphs with m edges and at most $m - k$ vertices, where k is a given nonnegative integer, then except when m is of the form $\binom{a}{2}$ and $k = \binom{a-1}{2} - 1$, the possible values for the quantity $\max\{d(p) + d(q) : pq \in E(G_0)\}$ is $m - k + 1, \ldots, m + 1$.

In principle, we can find out all the maximal graphs G that satisfy $\max\{d(p) + d(q) : pq \in E(G)\} = m + 1 - j$ for $j = 0, \ldots, k$ (using Lemma 4.3 or Corollary 4.4), rule out some of them (by using Theorem 3.6 or Theorem 3.9), and then compare the signless Laplacian spectral radii of the remaining ones to determine the graphs that maximize the signless Laplacian over all graphs with m edges and at most $m - k$ vertices. Of course, in practice, this is feasible only when k is small.

In below we demonstrate the method by giving the solution to the problem for $k = 0, 1, 2, 3$. For each fixed k, it suffices to give the maximal graphs that maximize the signless Laplacian spectral radius over all graphs with m edges and at most $m - k$ vertices. If G_0 is an optimal graph with m edges and n vertices, and $n < m - k$, then $G_0 \cup K_1^c, G_0 \cup K_2^c, \ldots, G_0 \cup K_{m-k-n}^c$ are also optimal graphs for the problem. We have the following results:

Theorem 4.6. *For every positive integer $m \geqslant 4$, $C(m - 3, 2, 1)$ is the unique graph that maximizes the signless Laplacian spectral radius over all graphs with m edges and at most m vertices.*

Theorem 4.7. *For $m \geqslant 5$, there is a unique maximal graph that maximizes the signless Laplacian spectral radius over all graphs with m edges and at most $m - 1$ vertices. For $m = 5$ (respectively, $m = 6$), the optimal graph is $C(2, 2)$ (respectively, K_4). For $m \geqslant 7$ the optimal graph is $C(m - 5, 2, 1, 1)$.*

Theorem 4.8. *The complete graph K_4 is the unique graph that maximizes the signless Laplacian spectral radius over all graphs with six edges and at most four vertices. There are precisely two graphs, namely,*

$C(1,3,1)$ and $C(3,2)$, that maximize the signless Laplacian spectral radius over all graphs with seven edges and at most five vertices. For $m \geqslant 8$, there are precisely two graphs, namely, $C(m-6,3,1)$ and $C(m-7,3,1,1)$ that maximize the signless Laplacian spectral radius over all graphs with m edges and at most $m-2$ vertices.

Theorem 4.9. *$C(1,2,2)$ (respectively, $C(4,2)$) is the unique graph that maximizes the signless Laplacian spectral radius over all graphs with eight edges and at most five vertices (respectively, nine edges and at most six vertices). There are precisely two maximal graphs, namely, $C(1,4,1,1)$ and K_5, that maximize the signless Laplacian spectral radius over all graphs with* 10 *edges and at most seven vertices. For $m \geqslant 11$, $C(m-9,4,1,1)$ is the unique graph that maximizes the signless Laplacian spectral radius over all graphs with m edges and at most $m-3$ vertices.*

In below we are going to provide a unified treatment for Theorems 4.6–4.9. Let G_0 denote a connected graph with m edges and n vertices that maximizes the signless Laplacian spectral radius over all graphs with m edges and at most $m-k$ vertices, where k is a fixed nonnegative integer less than or equal to 3.

By Corollary 4.4(i), if $\max\{d(p)+d(q) : pq \in E(G_0)\} = m+1$, then G_0 is equal to K_2, K_3 or is of one of the following forms: $C(n_1,n_2,1,1)$, $C(n_1,1)$, $C(n_1,2,1)$, $C(n_1,2)$. We rule out the possibility $G_0 = K_2$ (for $k = 0,\ldots,4$) as K_2 has more vertices than edges. For a similar reason, the graph $C(n_1,1)$ is also ruled out. The graph K_3 is also ruled out, except when $k = 0$.

Consider the possibility $G_0 = C(n_1,n_2,1,1)$. Note that $\delta_2+\delta_3 = 2+(n_2+1) = n_2+3$. But $n+1 = n_1+n_2+3$, so we always have $\delta_2+\delta_3 < n+1$, and by Theorem 3.6 we can find a maximal graph H with the same number of edges as G_0 but with one vertex more such that $\rho(Q(G_0)) < \rho(Q(H))$. If $n < m-k$ then the optimality of G_0 is violated. So in this case we must have $n = m-k$. For $k = 0$, the condition $n = m-k$ will lead to $n_2 = 1$, which is a contradiction. For $k = 1$, the condition gives $n_1 = m-5$ and so $G_0 = C(m-5,2,1,1)$. For $k = 2$, the condition $n = m-k$ yields $G_0 = C(m-7,3,1,1)$, For $k = 3$, we obtain $G_0 = C(m-9,4,1,1)$.

Consider the possibility $G_0 = C(n_1,2)$. Since $C(n_1,2)$ has precisely two dominating vertices, by Theorem 3.6 we can find a maximal graph H with m edges and $n+1$ vertices such that $\rho(Q(G_0)) < \rho(Q(H))$. By the optimality of G_0, we must have $n = m-k$. For $k = 0$, the latter condition implies $n_1 = 1$, which is not allowed. For $k = 1$, the condition yields $G_0 = C(2,2)$. For $k = 2,3$, we obtain $G_0 = C(3,2)$ and $G_0 = C(4,2)$ respectively.

If $G_0 = C(n_1,2,1)$ then m,n are both equal to n_1+3. For $k = 0$, this leads to $G_0 = C(m-3,2,1)$. For $k = 1,2,3$, this possibility cannot happen.

Consider the case $\max\{d(p)+d(q) : pq \in E(G_0)\} = m$. Then $k = 1, 2$ or 3. By Corollary 4.4(ii), G_0 equals K_4 or is one of the following forms: $C(n_1,n_2,2,1,1)$, $C(n_1,3,1)$, $C(n_1,2,2)$.

Consider the possibility $G_0 = C(n_1,n_2,2,1,1)$. For $i = 3$ and $l = 1$, we have $\delta_i+\delta_{r+1-i} = 2\delta_3 = 6$ and $\delta_l+\delta_{r-l}+1 = \delta_1+\delta_4+1 = 1+(n_2+3)+1 = n_2+5 \geqslant 6$. By Theorem 3.9 there is a maximal graph H with the same number of vertices and edges as G_0 such that $\rho(Q(H)) > \rho(Q(G_0))$, which contradicts the optimality of G_0. So this case cannot happen at all.

If $G_0 = C(n_1,3,1)$ then $n = m-2$. For $k = 1$, we rule out this possibility by applying Theorem 3.6 (with $i = 2$). For $k = 2$, we obtain $G_0 = C(m-6,3,1)$. For $k = 3$, this possibility clear cannot happen.

Consider the possibility $G_0 = C(n_1,2,2)$. In this case, $n = n_1+4$ and $m = 2n_1+6$. So we have $(m-k)-n = n_1+2-k > 0$, i.e., $n < m-k$, for $k = 1,2$, and $k = 3$ with $n_1 > 1$. Since $C(n_1,2,2)$ has precisely two dominating vertices, by Theorem 3.6 for $k = 1,2$ and $k = 3$ with $n_1 > 1$ such possibility is ruled out. What is left for this possibility is $G_0 = C(1,2,2)$ (when $k = 3$).

Since K_4 has six edges and four vertices, the possibility $G_0 = K_4$ can happen only for $k = 1,2$.

Consider the case $\max\{d(p)+d(q) : pq \in E(G_0)\} = m-1$. Then $k = 2$ or 3. By Corollary 4.4(iii), G_0 is $C(2,3)$ or is of one of the following forms:

$$C(n_1,n_2,2,1,1,1),\ C(n_1,2,2,1) \text{ or } C(n_1,2,1,2).$$

For the maximal graph $C(n_1,n_2,2,1,1,1)$ we have $\delta_3+\delta_4 = 7 < 7+n_2 = \delta_1+\delta_5+2$. So by Theorem 3.10 (with $i = 3$ and $l = 1$) G_0 cannot be of the form $C(n_1,n_2,2,1,1,1)$.

For the maximal graph $C(n_1, 2, 2, 1)$, we have $m = n_1 + 9$ and $n = n_1 + 5$; so $n < m - 3$. As $\delta_2 + \delta_3 = 3 + 4 = 7 \leqslant n + 1$, by Theorem 3.6 (with $i = 2$) we rule out the possibility $G_0 = C(n_1, 2, 2, 1)$.

For the maximal graph $C(n_1, 2, 1, 2)$, we have $m = 2n_1 + 9, n = n_1 + 5$ and so $m - n = n_1 + 4 \geqslant 5$. Since G_0 has two dominating vertices, by Theorem 3.6 we also rule out the possibility $G_0 = C(n_1, 2, 1, 2)$.

Finally, we consider the case $\max_{pq\in E(G_0)}\{d(p) + d(q)\} = m - 2$. Then $k = 3$. By Corollary 4.4(iv) G is of one of the following forms:

$$C(n_1, n_2, 3, 1, 1, 1), C(n_1, n_2, 3, 1, 1), C(n_1, 3, 2, 1), C(n_1, 4, 1),$$
$$C(n_1, 3, 1, 2), C(n_1, 3, 2), C(3, 3) \text{ or } K_5.$$

For the maximal graph $C(n_1, n_2, 3, 1, 1, 1)$, the number of edges is greater than the number of vertices by $n_2 + 6$. By Theorem 3.6 (with $i = 3$) we rule out the possibility $G_0 = C(n_1, n_2, 3, 1, 1, 1)$.

We also rule out the possibility $G_0 = C(n_1, n_2, 3, 1, 1)$ by applying Theorem 3.6 (with $i = 3$).

We rule out the possibility $G_0 = C(n_1, 3, 2, 1)$ by applying Theorem 3.6 (with $i = 2$).

Since $C(n_1, 3, 1, 2)$ has precisely two dominating vertices and its number of edges is greater than its number of vertices by at least 5, by Theorem 3.6 we rule out also the possibility $G_0 = C(n_1, 3, 1, 2)$. For a similar reason, we also rule out the possibility $G_0 = C(n_1, 3, 2)$.

If $G_0 = C(n_1, 4, 1)$, then $m = n_1 + 10$ and $n = n_1 + 5$; so $m - n = 5$. Also, $\delta_2 = 4$ and $n + 1 = n_1 + 6$. Hence $2\delta_2 \leqslant n + 1$ if and only if $n_1 \geqslant 2$. By Theorem 3.6 (with $i = 2$) we rule out the possibility $G_0 = C(n_1, 4, 1)$ for $n_1 \geqslant 2$. What remains is the possibility $G_0 = C(1, 4, 1)$.

Proof of Theorem 4.6. From the preceding discussion, it is clear that G_0 must be $C(m - 3, 2, 1)$. So the desired conclusion follows. □

Proof of Theorem 4.7. From the preceding discussion, we find that the optimal graph G_0 can only be one of the following:

$$C(m - 5, 2, 1, 1)(m \geqslant 6), C(2, 2)(m = 5) \quad \text{and} \quad K_4(m = 6).$$

In the above list, $C(2, 2)$ is the only graph with five edges and at most four vertices. So $C(2, 2)$ is the unique maximal graph that maximizes the signless Laplacian spectral radius over graphs with five edges and at most four vertices.

By calculation we have

$$(\Delta + B)(C(1, 2, 1, 1)) = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 2 & 1 & 1 \\ 0 & 2 & 3 & 1 \\ 1 & 2 & 1 & 4 \end{bmatrix}$$

and $q_{C(1,2,1,1)}(x) = (x - 1)f(x)$, where $f(x) = x^3 - 9x^2 + 20x - 8$. But $f(5) = -8$ and $f(6) = 4$. So $q(x)$ has a root λ lying between 5 and 6. If $\rho(Q(C(1, 2, 1, 1))) \geqslant 6 = \rho(Q(K_4))$, then we have

$$\lambda + \rho(Q(K_4)) > 11 > 10 = \operatorname{tr}(\Delta + B)(C(1, 2, 1, 1)),$$

which is a contradiction as $Q(C(1, 2, 1, 1))$ is positive semidefinite. So we have $\rho(Q(K_4)) > \rho(Q(C(1, 2, 1, 1)))$. Hence, K_4 is the unique maximal graph that maximizes the signless Laplacian spectral radius over graphs with six edges and at most five vertices. It is also clear that for $m \geqslant 7$, $C(m - 5, 2, 1, 1)$ is the unique graph that maximizes the signless Laplacian spectral radius over graphs with m edges and at most $m - 1$ vertices. □

Proof of Theorem 4.8. From the preceding discussion, we find that the optimal graph G_0 can only be one of the following:

$$C(3, 2)\ (m = 7), \quad C(m - 6, 3, 1)\ (m \geqslant 7), \quad C(m - 7, 3, 1, 1)\ (m \geqslant 8),$$
$$K_4(m = 6) \quad \text{or} \quad C(2, 3)\ (m = 9).$$

We are going to show that $\rho(Q(C(1, 3, 1))) = \rho(Q(C(3, 2))$. In fact, we can prove the following slightly more general result:

Assertion. $\rho(Q(C(1,3,n-4))) = \rho(Q(C(3,n-3)))$ for $n \geqslant 5$.

Proof of Assertion. By calculation we have

$$(\Delta + B)(C(3,n-3)) = \begin{bmatrix} n-3 & n-3 \\ 3 & 2n-5 \end{bmatrix} \quad \text{and}$$
$$(\Delta + B)(C(1,3,n-4)) = \begin{bmatrix} n-4 & 0 & n-4 \\ 0 & n & n-4 \\ 1 & 3 & 2n-6 \end{bmatrix}.$$

Moreover,

$$q_{C(3,n-3)}(x) = x^2 + (8-3n)x + 2n^2 - 14n + 24$$

and

$$\begin{aligned} q_{C(1,3,n-4)}(x) &= x^3 + (10-4n)x^2 + (5n^2 - 28n + 40)x + (-2n^3 + 18n^2 - 52n + 48) \\ &= [x - (n-2)]q_{C(3,n-3)}(x). \end{aligned}$$

But $\rho(K(C(3,n-3))) > n-2$, it follows that $\rho(Q(C(1,3,n-4)) = \rho(Q(C(3,n-3)))$.

Next, we show that $\rho(Q(C(m-6,3,1))) = \rho(Q(C(m-7,3,1,1)))$ for $m \geqslant 8$, and also $\rho(Q(C(3,3,1))) > \rho(Q(C(2,3)))$.

Straightforward calculations yield the following

$$(\Delta + B)(C(2,3)) = \begin{bmatrix} 3 & 3 \\ 2 & 6 \end{bmatrix}, \quad q_{C(2,3)}(x) = x^2 - 9x + 12,$$
$$(\Delta + B)(C(2,3,1,1)) = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 2 & 1 & 1 \\ 0 & 3 & 4 & 1 \\ 2 & 3 & 1 & 6 \end{bmatrix},$$

and

$$q_{C(2,3,1,1)}(x) = (x-1)p(x),$$

where $p(x) = x^3 - 12x^2 + 35x - 12$. Denote $\rho(K(C(2,3)))$ by ρ. Then ρ is the largest root of the polynomial $x^2 - 9x + 12$. A little calculation shows that the latter is approximately 7.372. By division, we have $p(x) = (x-3)(x^2 - 9x + 12) - 4(x-6)$. So $p(\rho) = -4(\rho - 6) < 0$. Hence the largest root of $p(x)$ is greater than ρ. This proves that $\rho(Q(C(2,3,1,1))) > \rho(Q(C(2,3)))$. By [14, Lemma 5.6] we have $\rho(Q(C(m-6,3,1))) = \rho(Q(C(m-7,3,1,1)))$ for $m \geqslant 8$. In particular, $\rho(Q(C(3,3,1))) = \rho(Q(C(2,3,1,1)))$. Hence, $\rho(Q(C(3,3,1))) > \rho(Q(C(2,3)))$.

We can now draw the desired conclusions. $\square$

Proof of Theorem 4.9. From the preceding discussions, we find that possible candidates for G_0 include:

$$C(1,2,2), C(4,2), C(m-9,4,1,1), C(2,3), C(1,4,1), C(3,3) \text{ and } K_5.$$

In the above list, $C(1,2,2)$ is the only graph with eight edges and at most five vertices. So $C(1,2,2)$ is the unique graph that maximizes the signless Laplacian spectral radius over all graphs with eight edges and at most five vertices.

The above list contains only two maximal graphs with nine edges and at most six vertices, namely, $C(4,2)$ and $C(2,3)$. We are going to compare $\rho(Q(C(4,2)))$ with $\rho(Q(C(2,3)))$.

By definition, the reduced signless Laplacian of $C(2,3)$ is given by: $(\Delta + B)(C(2,3)) = \begin{bmatrix} 3 & 3 \\ 2 & 6 \end{bmatrix}$. So the reduced signless Laplacian characteristic polynomial $q_{C(2,3)}(x)$ of $C(2,3)$ is $x^2 - 9x + 12$. According to Theorem 2.1, $\rho(Q(C(2,3)))$ is equal to $\frac{9+\sqrt{33}}{2}$, the largest root of $x^2 - 9x + 12$. Similarly, $\rho(Q(C(4,2))$ is equal to the largest root of $q_{C(4,2)}(x)$, which is $x^2 - 8x + 4$; that is, $\rho(Q(C(4,2)) = \frac{8+\sqrt{48}}{2}$. By comparison, we find that $\rho(Q(C(4,2)))$ is larger. So $C(4,2)$ is the unique graph that maximizes the signless Laplacian spectral radius over all graphs with nine edges and six vertices or less.

The above list also contains only two maximal graphs with 10 edges and at most seven vertices, namely, $C(1,4,1,1)$ and K_5. In general, $\rho(Q(K_n)) = 2n-2$; so $\rho(Q(K_5)) = 8$. To compute $\rho(Q(C(1,4,1,1)))$, we consider the reduced signless Laplacian of $C(1,4,1,1)$, which is given by:

$$(\Delta + B)(C(1,4,1,1))) = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 2 & 1 & 1 \\ 0 & 4 & 5 & 1 \\ 1 & 4 & 1 & 6 \end{bmatrix}.$$

It is readily checked that the positive vector $(1,2,5,7)^T$ is an eigenvector of the latter matrix corresponding to 8. So $\rho(Q(C(1,4,1,1)))$ is also equal to 8. We can now conclude that altogether there are precisely two maximal graphs that maximize the signless Laplacian spectral radius over all graphs with 10 edges and at most seven vertices, namely, $C(1,4,1,1)$ and K_5.

The above list contains also $C(2,4,1,1)$ and $C(1,4,1)$ as the only maximal graphs with 11 edges and at most eight vertices. Let us compare their signless Laplacian spectral radii. Straightforward calculations give

$$(\Delta + B)(C(2,4,1,1)) = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 2 & 1 & 1 \\ 0 & 4 & 5 & 1 \\ 2 & 4 & 1 & 7 \end{bmatrix}, \quad (\Delta + B)(C(1,4,1)) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 7 & 1 \\ 1 & 4 & 5 \end{bmatrix}$$

and

$$q_{C(2,4,1,1)}(x) = (x-1)(x^3 - 14x^2 + 48x - 32) \quad \text{and} \quad q_{C(1,4,1)}(x) = (x-4)(x^2 - 9x + 6).$$

Denote $\rho(Q(C(1,4,1)))$ by ρ. According to Theorem 2.1, ρ is equal to the largest (real) root of $q_{C(1,4,1)}(x)$. But $\rho > d_{\max}(C(1,4,1)) + 1 = 6$, so we have $\rho^2 - 9\rho + 6 = 0$. For a similar reason, $\rho(Q(C(2,4,1,1)))$ is the largest (real) root of $f(x)$, where $f(x) = x^3 - 14x^2 + 48x - 16$. By division, we have $f(x) = (x^2 - 9x + 6)(x - 5) - 3x + 14$ and so $f(\rho) = -3\rho + 14 < 0$. Hence, the largest root of $f(x)$ must be greater than ρ. This proves that $\rho(Q(C(2,4,1,1))) > \rho(Q(C(1,4,1)))$.

The above list contains $C(3,4,1,1)$ and $C(3,3)$ as the only maximal graphs with 12 edges and at most nine vertices. We are going to rule out $C(3,3)$ by showing that its signless Laplacian spectral radius is less than that of $C(3,2,2)$. Note that the maximal graph $C(3,2,2)$ itself does not maximize the signless Laplacian spectral radius over all graphs with 12 edges and at most nine vertices, as $C(3,2,2)$ has seven vertices and 12 edges, and it has precisely two dominating vertices. By calculation we find that

$$q_{C(3,2,2)}(x) = (x-3)q_{C(3,3)}(x) - 12x + 12.$$

Denote $\rho(Q(C(3,3)))$ by ρ and note that $\rho > 6$. Then $q_{C(3,2,2)}(\rho) = -2\rho + 12 < 0$. It follows that we have $\rho(Q(C(3,2,2))) > \rho(Q(C(3,3)))$, as desired.

Finally, for $m \geqslant 13$, $C(m-9,4,1,1)$ is the only maximal graph in the above list with m edges and $m-3$ vertices. We can now conclude that for $m \geqslant 11$, $C(m-9,4,1,1)$ is the unique graph that maximizes the signless Laplacian spectral radius over all graphs with m edges and at most $m-3$ vertices. The proof is complete. $\square$

The conjecture given in [22, Problem AWGS.9.], mentioned at the introductory section, roughly says that for $3 \leqslant k \leqslant n-4$ if G maximizes the spectral radius of the adjacency matrix over the set of all connected graphs with n vertices and $n+k$ edges then G is either $G_{n,k}$ or $H_{n,k}$. In our notation, $G_{n,k}$, $H_{n,k}$ are the maximal graphs given by:

$$G_{n,k} = \begin{cases} C(n-d-1, d, 1) & \text{if } t = 0, \\ C(n-d-2, 1, d-t, t, 1) & \text{if } 1 \leqslant t \leqslant d-2, \\ C(n-d-2, 2, d-1, 1) & \text{if } t = d-1, \end{cases}$$

where t, d are the unique integers that satisfy $k+1 = \binom{d}{2} + t$, $0 \leqslant t \leqslant d-1$, and

$$H_{n,k} = \begin{cases} C(n-3,2,1) & \text{if } k=0, \\ C(n-k-3,k+1,1,1) & \text{if } 1 \leqslant k \leqslant n-4, \\ C(2,n-2) & \text{if } k=n-3. \end{cases}$$

We have been able to establish the following corresponding result for the signless Laplacian spectral radius: For $3 \leqslant k \leqslant n-3$, $H_{n,k}$ is the unique graph that maximizes the signless Laplacian spectral radius among all connected graphs with n vertices and $n+k$ edges. The result will be published in our future work.

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